Chemistry Physics and Biology of Colloids and Interfaces

15-19 June 2025 Eger, Hungary

BOOK OF ABSTRACTS

	Sunday 15. June	Monday 16. June	Tuesday 17. June	Wednesday 18. June	Thursday 19. June
9.00-9.30		Laage	Monopoli	Pankhurst	Dong
9.30-9.50					László
9.50-10.10		Kővágó	Voniatis	Bilous	Sajdik
10.10-10.30		Tóth Ugyonka	Turcsányi	Halmóczki	Matias
10.30-11.00		Coffee break	Coffee break	Coffee break	Coffee break
			Zrinyi	Bányai	Kónya
11.10-11.40		Hollóczki	M. Chen	Kovač	
11.40-12.00		Kaszab	Manikion	Novák	Mao
12.00-12.20		Liu	Molnár	Szabó	Kóth
12.20-12.40		Prikler	Zs. D. Kónya	Kéri	Y. Chen
12.40-13.00		Zhao	Pálos	Júlio Santos	CLOSING
13.00-14.30		Lunch	Lunch	Lunch	Lunch
14.30-15.20		Allen	Figueiredo	Kantorovich	
15.20-15.50		Coffee break	Coffee break	Coffee break	
15.50-16.20		POSTER SESSION	Kellermayer	Mihály	
16.20-16.40			Lei	Seres	
16.40-17.00			Mostarac	Budavári	
17.00-17.20			João Santos	Terefe	
17.20-18.00					
18.10-18.30	OPENING				
18.30-19.00	Bain				
19.00-19.20					
19.20-21.30	GET TOGETHER PARTY	Wine tasting (optional)		CONFERENCE DINNER	
21.30-22.00					

Conference Program

Sunday, 15 June

14.00-18.00 Registration (in Hotel Eger & Park)

18.10-18.30: Conference opening

Session 1 (chair: Pál Jedlovszky):

18.30-19.20: **Colin Bain** (Durham, UK): *(Mis)-conceptual frameworks in colloid and interface science*

19.20-21.30: Welcome reception

Monday, 16 June

Session 2 (chair: Sofia Kantorovich):

09.00-09.50: **Damien Laage** (Paris, France): *Acidity of the air-water interface: excess proton thermodynamics, dynamics and spectroscopy*
09.50-10.10: **Bence Kővágó** (Vienna, Austria): *Polymers at the air-water interface*
10.10-10.30: **Helga Tóth Ugyonka** (Eger, Hungary): *Computer Simulation Investigation of the Molecular Scale Structure and Dynamics of the Free Surface of Imidazolium-Based Ionic Liquids*

10.30-11.10: Coffee break

Session 3 (chair: Mónika Kéri):

11.10-11.40: **Oldamur Hollóczki** (Debrecen, Hungary): *Modeling the effects of microplastics on biomolecular systems*
11.40-12.00: **Edit Kaszab** (Gödöllő, Hungary): *Microplastics and heavy metals in sewage sludge and the effect of their co-occurrence on* Pseudomonas aeruginosa
12.00-12.20: **Quian Liu** (Aarhus, Denmark): *S100B chaperone modulates phenol-soluble modulin amyloid formation in* Staphylococcus aureus *biofilm*
12.20-12.40: **Bence Prikler** (Gödöllő, Hungary): *Quantifying Biofilm Formation on Different Plastic Surfaces*
12.40-13.00: **Guansen Zhao** (London, UK): *Thermal transport and coupling effects in molecular liquids and aqueous solutions under thermal gradients*

13.00-14.30: Lunch

Session 4 (chair: Damien Laage):

14.30-15.20: **Heather Allen** (Columbus, USA): *Aqueous Interfaces: Molecular and Ion Organization*
15.20-15.50: Coffee break

15.50-18.30: POSTER SESSION

19.00-22.00: Wine tasting (optional event)

Tuesday, 17 June

Session 5 (chair: Miklós Kellermayer):

09.00-09.50: **Marco Monopoli** (Dublin, Ireland): *Understanding the nanomaterial interaction with biomolecules, a journey from safety to healthcare applications*
09.50-10.10: **Constantinos Voniatis** (Budapest, Hungary): *Nanofibrous dual polymer meshes for surgical tissue regeneration*
10.10-10.30: **Árpád Turcsányi** (Szeged, Hungary): *Bimetallic nanoclusters: Synthesis optimization and biological studies*

10.30-11.00: Coffee break

Session 6 (chair: Judith Mihály):

11.00-11.20: **Miklós Zrínyi** (Budapest, Hungary): *Mechanical Behaviour of Fibrous Materials*
11.20-11.40: **Menglin Chen** (Aarhus, Denmark): *Electrohydrodynamics based Functional Fibers for Wireless Neuromodulation*
11.40-12.00: **Kenigen Manikion** (Budapest, Hungary): *Fabrication, Degradation Dynamics and Mechanical Integrity of Advanced Composite Electrospun Meshes*
12.00-12.20: **Kristóf Molnár** (Budapest, Hungary): *Synthesis and properties of hydrogel fibers*
12.20-12.40: **Zsuzsanna Kónya** (Szeged, Hungary): *Co-immobilization of protease enzyme and molecular antioxidant on anionic clays*
12.40-13.00: **Veronika Pálos** (Budapest, Hungary): *Polysuccinimide-based electrospun scaffolds loaded with different salts for potential use in wound dressings*

13.00-14.30: Lunch

Session 7 (chair: Marco Monopoli):

14.30-15.20: **Antonio Figueiredo Neto** (São Paulo, Brazil): *Oxidative Stress and Lipid Profile During Acute Phase of COVID-19 Infection and After Recovery: Evidence of a Sequel in LDL*

15.20-15.50: Coffee break

15.50-16.20: **Miklós Kellermayer** (Budapest, Hungary): *Single-molecule mechanics of chemically modulated DNA*
16.20-16.40: **Li Lei** (London, UK): *Molecular Dynamics simulation of adsorption and aggregation of therapeutic antibody fragments at water-oil interfaceees*
16.40-17.00: **Deniz Mostarac** (Vienna, Austria): *Influence of Crowders and Ligands on the Polymeric Properties of G-Quadruplex Multimers*
17.00-17.20: **João Santos** (Coimbra, Portugal): *Host–Guest Chemistry of β-Cyclodextrin with Platinum(II) Drugs: Inclusion Complex Formation and Cytotoxic Profiles*

Wednesday, 18 June

Session 8 (chair: Angéla Jedlovszky-Hajdú):

09.00-09.50: **Quentin Pankhurst** (London, UK): *Some recent developments in magnetic field hyperthermia: from standards to clinical studies*
09.50-10.10: **Oksana Bilous** (Vienna, Austria): *Self-diffusion and clustering phenomena in magnetically controlled ferrogranulate system*
10.10-10.30: **Sarolta Halmóczki** (Budapest, Hungary): *Development of Electrospun Wound Healing Matrices Using Metal Nanoparticles*

10.30-11.00: Coffee break

Session 9 (chair: Zoltán Kónya):

11.00-11.20: **István Bányai** (Debrecen, Hungary): *NMR for Colloids: Achievements and Pitfalls*
11.20-11.40: **Jure Kovač** (Ljubljana, Slovenia): *From Hydrogen to Fluorine: Structural and Dynamic Consequences in Alcohols Explored by MD and SWAXS*
11.40-12.00: **Levente Novák** (Debrecen, Hungary): *Relaxivity properties of paramagnetic metal ion complexes with polymers synthesized from smaller building blocks*
12.00-12.20: **Tamás Szabó** (Szeged, Hungary): *Ultrasonic fracture and dispersion of regular and novel carbon nanostructures: from graphite to soft mesoporous graphene frameworks*
12.20-12.40: **Mónika Kéri** (Debrecen, Hungary): *Swelling and structure of biodegradable crosslinked polyurethanes by NMR*
12.40-13.00: **Júlio Santos** (Budapest, Hungary): *Molecular dynamics simulations of Magneto-active elastomers*

13.00-14.30: Lunch

Session 10 (chair: Oldamur Hollóczki):

14.30-15.20: **Sofia Kantorovich** (Vienna, Austria): In silico *investigations of magnetic soft matter*

15.20-15.50: Coffee break

15.50-16.10: **Judith Mihály** (Eger, Hungary): *Extracellular vesicles detection via surface enhanced IR spectroscopy using plasmonic gold nanoparticles*
16.10-16.30: **László Seres** (Szeged, Hungary): *Liposomal formulations of flavonoids*
16.30-16.50: **Bálint Budavári** (Eger, Hungary): *Budesonide-loaded liposomes for inhalation*
16.50-17.10: **Abelneh Terefe** (Nagykanizsa, Hungary): *The Effect of Surfactants on Polyelectrolyte Multilayer Nanofiltration Membranes*

18.00-22.00: Conference banquet

Thursday, 19 June

Session 11 (chair: István Szilágyi):

09.00-09.30: **Mingdong Dong** (Aarhus, Denmark): *Controlled Self-Assembly and Disassembly of Amyloid Peptide Crystals*
09.30-09.50: **Krisztina László** (Budapest, Hungary): *3D plasma assisted adsorptive removal of organic pollutants from water by porous carbon*
09.50-10.10: **Kadosa Sajdik** (Szeged, Hungary): *Water Pollution Mitigation by Removal of Local Anesthetics via Liquid-phase Adsorption on Graphene Oxide*
10.10-10.30: **Pedro Matias** (Coimbra, Portugal): *From powder to beads: insights into an imine-linked triazine porous organic polymer for the remediation of fluoroquinolone antibiotics from water*

10.30-11.00: Coffee break

Session 12 (chair: Pál Jedlovszky):
11.00-11.50: **Zoltán Kónya** (Szeged, Hungary): *Surfaces and interfaces in heterogeneous catalysis*
11.50-12.10: **Meng Mao** (Harbin, China): *Swimming nanorobots for targeted therapy in glioblastoma treatment*
12.10-12.30: **János Kóth** (Budapest, Hungary): *Visible Light Photocatalytic-Adsorption Effect of Recyclable Industrial Waste*
12.30-12.50: **Yong Mei Chen** (Xi'an, China): *Tough gel based ionotronics for flexible electronics*

12.50-13.15 Conference closing

13.10-14.30: Lunch

List of Posters

1. **Márton Ács** (Budapest, Hungary): *Freeze-dried liposomes for inhalation*
2. **Orsolya Adamcsik** (Nagykanizsa, Hungary): *Comparative analysis of virus nucleic acid extraction methods from wastewater samples*
3. **Bálint Alács** (Budapest, Hungary): *Characterization of immobilased enzyme kinetics on magnetic nanoparticles*
4. **Mónika Bak** (Budapest, Hungary): *Structuring liquids through solvent-assisted interfacial association of oppositely charged polyelectrolytes and amphiphiles*
5. **Bálint Bakk** (Szeged, Hungary): *Role of Fluorocarbon Chain Length in the Adsorption of Perfluoroalkyl Substances on Nanoplastic Particles*
6. **Christodoulos Chrysanthou** (Budapest, Hungary): *Fabrication of poly (amino acid) based meshes for enhanced postoperative pain relief*
7. **Viktória Cseh** (Szeged, Hungary): *Monolayer-forming properties of bovine serum albumin and its composite multilayers on solid surfaces*
8. **Zhibo Deng** (London, UK): *Modeling Asymmetry in Flat Bilayers and Exosome-Like Vesicles: A Focus on Cholesterol Dynamics under Temperature Gradients*
9. **Eszter Fabó** (Budapest, Hungary): *Development and Characterization of Fiber-Reinforced Biodegradable Packaging Materials*
10. **Evelin Forró** (Budapest, Hungary): *Multi-Scale Mechanics of Cryopreserved Human Arterial Allografts Across a Six-Month Period*
11. **Dániel Fülöp** (Budapest, Hungary): *Fluidic Synthesis of Cationic Carbon Quantum Dots: Investigating Reaction Mechanism and Fluorescence Properties*
12. **Melkamu Birlie Genet** (Nagykanizsa, Hungary): *Magnetite-reduced graphene oxide nanocomposite for the simultaneous removal of bisphenol A and glyphosate from aqueous solutions*
13. **Adél Hordós** (Budapest, Hungary): *Fabrication and Mechanical Characterization of Polymer Fiber Systems in Physiologically Relevant Environment*
14. **Marius Horváth** (Budapest, Hungary): *Biocompatible composite protective thin layer using sol-gel chemistry*
15. **Erzsébet Illés** (Szeged, Hungary): *Polycarboxylate coated Ni ferrite nanomagnets and the bio nano interface*
16. **László Janovák** (Szeged, Hungary): *Development of hydrophobically modified chitosan-pluronic nanoparticles for sustained and targeted drug release in ischemic brain tissues*
17. **Byung Suk Jin** (Seoul, South Korea): *Shear-induced catastrophic phase inversion of high oil content O/W emulsions*
18. **Agaya Johnson** (Vienna, Austria): *Coarse-grained simulations of peptide $LGE1_{1-80}$*

19. **Dorottya Kis** (Budapest, Hungary): *Development of coaxial electrospun PSI fibers containing zinc and strontium salts for wound dressing application*
20. **Enikő Krisch** (Budapest, Hungary): *Poly(aspartic acid) hydrogels with Priamine^{TM} 1075 as a crosslinker*
21. **Krisztina László** (Budapest, Hungary): *Binding characteristics of fluorescent probes to pillararene modified graphene oxide nanosheets and their implications for indicator displacement assays*
22. **Lerato Emelda Mothoa** (Gödöllő, Hungary): *Microbial colonization and phenotypic resistance profile investigation across common polymer types*
23. **Zoltán Murányi** (Eger, Hungary): *New process for producing nanosilver*
24. **Gréta Papp** (Szeged, Hungary): *Biopolymer-enhanced viscosity in salt solutions: effect of inorganic and organic cations*
25. **Noémi Péli** (Budapest, Hungary): *Enzyme Replacement Therapy via Silica-Immobilized Human Tyrosine Hydroxylase*
26. **András Rázsi** (Eger, Hungary): *Connections between the spread of respiratory diseases and the weather*
27. **Vivien Rizmajer** (Budapest, Hungary): *Preparation of Magnetite-Containing Polymer Wound Dressing by Electrospinning*
28. **Kadosa Sajdik** (Szeged, Hungary): *Colloidal (de)stabilization of graphene nanoplatelets using graphene oxide*
29. **Salman Shabbir** (Veszprém, Hungary): *$CaCl_2$ transport in nanopores: competition of ions and water at the charged surface groups and the effect of charge scaling on selectivity*
30. **Tamás Stummer** (Budapest, Hungary): *Engineered magnetic nanoparticles as advanced carrier materials for enzyme catalyst*
31. **Donát Szalai** (Budapest, Hungary): *Investigation of pH-dependent swelling of nanohydrogel fibrous fibers*
32. **Kata Szayly** (Budapest, Hungary): *Characterization of mucoadhesion of polymer tablets on a hydrogel surface applying tensile and shear stress*
33. **Viktor Szilágyi** (Budapest, Hungary): *Simulation-assisted Electrostatic Fibre Formation and Cellular Adhesion into the Nanofibre Structure*
34. **Ildikó Y. Tóth** (Szeged, Hungary): *Wetting end evaporation on CNT- and ZnO-forests*
35. **Dániel Viczián** (Szeged, Hungary): *Effects of electrolytes and polyelectrolytes on the colloidal stability and enzyme-like activity of CeO_2 nanozymes*
36. **Attila Vörös** (Szeged, Hungary): *Papain functionalized Prussian blue nanozyme colloids of triple enzymatic function*
37. **Chao Zeng** (London, UK): *Interfacial thermal conductance of Janus nanoparticles*
38. **Anna Zrinyi** (Budapest, Hungary): *Development of selective sol-gel enzyme immobilization methods on magnetic nanoparticles*

Invited lectures

Aqueous Interfaces: Molecular and Ion Organization

Heather C. Allen, Biswajit Biswas, Gwen Gattermeir, Tai Bowling-Charles, Jovica Badjic, Shamma Proma, Narendra Adhikari

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ABSTRACT

Biomembrane ion transfer, lung surfactant, energy applications, ocean to marine aerosol concentration enrichments and aerosol-surface electric fields, phosphate capture, drug delivery molecular-systems, and environmental nanoplastics provide much motivation for studies of interfacial ion pairing, binding, and surface prevalence and organization of molecules and ions at interfaces. Ion surface activity and organization at aqueous soft interfaces has been controversial for decades. Here interfacial structure and the interfacial driving forces are presented using vibrational sum frequency generation spectroscopy (VSFG), second harmonic generation (SHG), Brewster angle microscopy (BAM), surface potential, surface tension, polarized Raman, and reflection absorption infrared spectroscopy. The focus of the presented work is on Mg(II), Fe(III), Al(III), SO_4^{2-} and other co-ions and water in which ion surface prevalence is inferred. Additionally, surfactants, phospholipids and synthesized molecular baskets at interfaces are studied; binding mechanisms are revealed in which driving forces of electrostatics and nonspecific dispersion compete. Molecular basket design is optimized for interfacial activity and binding affinity toward bio-target ions. Additionally, work on nanoplastic-induced reorganization of ocean surface proxy films and subsequent impact is discussed.

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[4] Vazquez de Vasquez, M., Rudd, M., Baer, M., Beasley, Emma, E., Allen, H.C. “Role of Hydration in Magnesium versus Calcium Ion Pairing with Carboxylate: Solution and the Aqueous Interface”, *Phys. Chem. B* V125, 40, 11308, (2021).

(Mis)-conceptual frameworks in colloid and interface science

Colin D. Bain

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ABSTRACT

Colloid and Interface Science uses both mathematical and conceptual frameworks. These conceptual frameworks – which are often deeply ingrained from our formative education – help us to make sense of the mathematics. But conceptual frameworks also condition the way we design experiments and constrain the explanations that we construct from experimental data. Resources such as Generative AI tend to reinforce canonical concepts in the training set used in the large language model and may encourage an uncritical acceptance of conceptual frameworks. A similar critique holds for pictures, that help us to understand concepts but often convey additional information that can mislead.

This talk will explore four examples that suggest the need for a more critical approach to core concepts widely used in colloid and interface science (and elsewhere):

(i) Rate constants for micellar processes. [1] [2]
(ii) Colloidal particles in flowing liquids [3]
(iii) The physical origin of electrical double layers
(iv) The Coulomb interaction in water

The first two examples will be illustrated from my own research on kinetics in surfactant systems and the drying of droplets on surfaces. The last two examples were stimulated by conversations with colleagues.

REFERENCES

[1] Griffiths, I. M.; Bain, C. D.; Breward, C. J. W.; Colegate, D. M.; Howell, P. D.; Waters, S. L., “On the Predictions and Limitations of the Becker–Döring Model for Reaction Kinetics in Micellar Surfactant Solutions”, J. Coll. Interface Science **360**, 662–671 (2011).
[2] Yan, C.; Angus-Smyth, A.; Bain, C. D., ”Adsorption Kinetics of Nonionic Surfactants in Micellar Solutions: Effects of Added Charge”, Faraday Discussions **160**, 45–61, (2013)
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Oxidative Stress and Lipid Profile During Acute Phase of COVID-19 Infection and After Recovery: Evidence of a Sequel in LDL

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ABSTRACT

This study aimed to investigate the atherogenicity (quality) of the Low-Density Lipoprotein (LDL) particles in patients with acute and recovered from COVID-19 infection. The participants were adults, aged 18 years or older of both sexes. Those with positive RT-PCR results at baseline were included in the Acute COVID-19 group (n = 33), and those with negative RT-PCR six months after acute infection, were included in the Recovered COVID-19 group (n = 30). The LDL quality was evaluated using three validated methods: Z-scan, UV–visible spectroscopy, and Lipoprint system. The Recovered COVID-19 group showed significantly higher numbers of large LDL particles (less atherogenic) than the Acute COVID-19 group ($P < 0.05$). We also found that COVID-19 infection was associated with the oxidative modification of LDL particles. D-dimer and CRP levels were correlated with Z-scan results and antioxidant-amount estimate. Moreover, we noticed that the infection left a sequel in LDL quality, even after six months of recovery. These findings highlight the importance of monitoring lipids during and after recovery from COVID-19 infection, and their potential deleterious effect on the LDL profile might correlate with the progression of atherosclerosis and poor clinical outcomes. In the talk we will discuss the use of nonlinear optical techniques to investigate biological structures, particularly the LDL. We will show that the nonlinear optical response from native and atherogenic LDL particles are different, and the Z-Scan technique can be applied to evaluate the risk of patients develop a cardio-vascular disease. Other pathologies, as periodontitis and diabetics, will be discussed in this framework.

REFERENCE

[1] Z. Lotfollahi, L. S. Neres, A. F. Mathias, M. C. P. Freitas, F. C. Cartolano, A. C. Varella, P. A. Lotufo, A. C. Goulart, N. R. T. Damasceno, J. B. Andrade, R. A. Fock, and A. M. Figueiredo Neto, “Oxidative Stress and Lipid Profile During Acute Phase of COVID-19 Infection and After Recovery: Evidence of a Sequel in LDL”, Brazilian Journal of Physics, **55**, 54 (2025).

In silico investigations of magnetic soft matter

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ABSTRACT

The development of magnetically responsive colloids with tuneable rheological properties at the nano- and micro-scale has garnered considerable interest, driving both experimental and theoretical advances [1]. A wide array of such systems has emerged, spanning from single-domain magnetic nanoparticles to complex assemblies such as multicore particles, where constituent grains exhibit internal magnetic anisotropy. These multicore architectures present unique challenges and opportunities in understanding and harnessing magnetic interactions at multiple scales.

While equilibrium properties of magnetic fluids, gels, and anisotropic colloids have been successfully captured via computational approaches [2-7], the dynamic behaviour—especially in systems featuring intrinsic magnetic anisotropy or complex internal structure—remains less understood. In particular, the influence of internal grain anisotropy on the collective dynamics of multicore particles, anisotropic nanoparticles, and hybrid materials like magnetic elastomers and polymer-like chains presents a rich and open area of study.

In this contribution, I will present a computational framework based on coarse-grained molecular dynamics simulations, incorporating three complementary approaches to model particle magnetism: the egg model [8,9], and the hot Stoner-Wohlfarth paradigm [10,11]. To account for solvent-mediated effects, the Lattice-Boltzmann method is employed to include hydrodynamic interactions. Emphasis will be placed on the role of internal anisotropy in shaping the dynamic behaviour of multicore particles, anisometric colloids, and magnetically functionalised soft materials. Our findings underscore the interplay between particle-level magnetic structure and collective dipolar interactions, offering new insights for the design of advanced magnetorheological materials.

REFERENCES

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[2] L. Rovigatti, J. Russo and F. Sciortino, *Phys. Rev. Lett.*, **2011**, *107*, 237801.
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Surfaces and interfaces in heterogeneous catalysis

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ABSTRACT

The support plays a crucial role in heterogeneous catalysis by providing mechanical stability to the active metal particles and actively influencing catalyst performance. Through **metal-support interactions (MSI)**, the support can alter the electronic properties, oxidation states, and dispersion of metal nanoparticles, directly impacting catalytic activity and selectivity. Reducible oxide supports often enhance these effects through charge transfer or oxygen mobility facilitating the formation of active sites. Beyond MSI, the surface structure, pore size, and crystallographic orientation of the support can guide the spatial distribution and morphology of metal particles during synthesis, ultimately affecting the reaction pathway and kinetics. By carefully selecting and engineering the support, it is possible to not only stabilize the active phase but also tailor the catalytic behavior toward enhanced efficiency and selectivity in targeted reactions.

We investigated the synergistic effects of metal-support interactions in CO_2 hydrogenation. A comprehensive characterization approach – including transmission electron microscopy (TEM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and in situ diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) – was employed to probe structural and chemical environments of the catalysts, monitor changes in oxidation states, and identify surface intermediates during reaction. The degree of metal-support interaction established in these systems was examined in the CO_2 hydrogenation – a model reaction selected for its simplicity, as it yields only two main products at ambient pressure (CO and CH_4). The catalytic performance was assessed in terms of CO_2 conversion and product selectivity.

In conclusion, the judicious choice and engineering of supports for metal nanoparticles are paramount to controlling metal-support interactions, which in turn dictate the catalytic activity and stability, ultimately enabling the design of novel and highly efficient catalysts for various applications.

Acidity of the air-water interface: excess proton thermodynamics, dynamics and spectroscopy

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ABSTRACT

The acidity of the air–water interface is a key determinant of chemical reactivity in atmospheric aerosols and at ocean surfaces. Yet, whether the water surface is more or less acidic than the bulk has long been debated. Here, we demonstrate how recent advances in machine-learned interatomic potentials enable accurate and efficient reactive molecular simulations, offering molecular-level insight into interfacial acid–base chemistry.

We will first discuss the thermodynamics of hydronium ion affinity for the interface, revealing that while the local hydronium concentration displays a gradient near the surface, the pH remains spatially uniform [1]. We will then correlate the simulated preferential surface adsorption of hydronium ions with experimental vibrational sum-frequency generation (vSFG) spectroscopy [2-3], and use direct computation of nonlinear vibrational spectra from our simulations to reveal the vibrational signature of interfacial hydronium ions [4]. Finally, we will characterize the dynamics of excess protons at the interface [5], contrast it with the bulk situation [6] and explain why Grotthuss proton diffusion is slower at the surface than in the bulk, even as water molecule diffusion is faster.

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Understanding the nanomaterial interaction with biomolecules, a journey from safety to healthcare applications

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ABSTRACT

For nanomedicine and nanosafety, there is a growing desire for a rational basis within which to understand nanoparticle-cell and organ level interactions. Nanoparticles in biological fluids (blood, or otherwise) generically associate with a range of biopolymers, especially proteins, organised into the 'biomolecular corona' which is continuously exchanging with the proteins in the environment. In some cases, the residence times of proteins in the corona are sufficiently long that they confer an effective biological identity onto the nanoparticle. The transport and fate of nanoparticles (from intracellular trafficking to clearance pathways) likely reflect the corona, rather than the nanomaterial itself.

It is now clear that these interactions lead to dramatic surface changes and a new identity of the NP in biological fluid and the corona can induce unpredictable immunological responses and can hamper their therapeutic efficacy.

The corona is derived from proteins in biological fluids, many of which are glycosylated. We have now demonstrated that the biomolecular corona exhibits a strong glycosylation component that is biologically active. This class of biomolecules plays a significant role in the NP colloidal stability and firmly controls the NP's biological fate. If controlled, this can offer new opportunities in nanomedicine.

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Some recent developments in magnetic field hyperthermia: from standards to clinical studies

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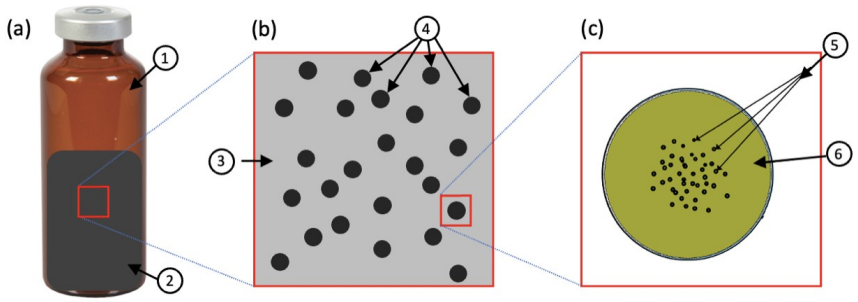
ABSTRACT

In magnetic field hyperthermia (MFH), a time-varying magnetic field $H(t) = H_o \sin(2\pi f t)$ is used to deliver thermal energy into implanted magnetic materials in the human body, for therapeutic purposes. Currently, MFH is used clinically in the treatment of glioblastoma and prostate cancer and is being tested for pancreatic cancer. It is also the subject of extensive *in vitro* and preclinical testing as researchers explore ways to optimise and use it.



Example of a magnetic fluid used in MFH. Key: 1 = glass vial; 2 = RCL Agent (magnetic fluid); 3 = supernatant of water for injection & saline; 4 = multicore magnetic nanoparticles; 5 = individual iron oxide cores; and 6 = dextran-40 matrix.

In this lecture a selection of recent examples of developments in MFH will be presented and discussed. The examples will include: • standardisation of the terminologies used in MFH [1]; • the introduction of ISO standards on the specification of characteristics and measurement methods for magnetic nanosuspensions and nanostructured beads [2]; • a review of the safety aspects of non-specific eddy current heating associated with MFH [3]; • a multi-site inter-laboratory study and review of challenges and recommendations for MFH characterisation measurements [4]; • the evaluation of deep-tissue MFH localisation methods using pulse sequencing [5,6]; and • the latest reports on a recently completed clinical study of MFH for the treatment of locally advanced pancreatic cancer [7].

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Keynote lectures

Controlled Self-Assembly and Disassembly of Amyloid Peptide Crystals

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Amyloid self-assembly is a complex phenomenon with implications for both degenerative human diseases and materials science. Among the diverse structures formed—fibers, particles, and crystals—amyloid crystals represent the most thermodynamically stable form. However, precise control over the assembly process and reversible manipulation of crystallization remain significant challenges. This study investigates the reversible formation of macroscopic amyloid crystals by systematically varying temperature, pH, ionic strength, and solvent conditions. In situ microscopy is employed to monitor the dynamics of amyloid disassembly in real time. The ability to induce reversible self-assembly through external stimuli offers new insights into the fundamental mechanisms governing amyloid crystallization and highlights the critical role of environmental factors. These findings may open new pathways for the rational design of dynamic biomaterials with tunable properties.

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Modeling the effects of microplastics on biomolecular systems

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ABSTRACT

Through the fragmentation of plastic waste, micro- and nanoplastics (MNPs) are formed and distributed through our environment. While these particles have been observed in food, various organisms, and even in human tissues, their impact is still unclear, partly due to the variety of MNPs in composition, size, shape, compounds at their surface (i.e., corona), and partly due to the limitations of analytical techniques to observe them.

In our efforts to utilize molecular modeling to provide a structural understanding on the environmental effects of MNPs, we established a simulated annealing molecular dynamics protocol to generate nanoplastic models for molecular simulations. With the aim to avoid needing to perform such a series of simulations each time before simulating a system that contains nanoplastics, we created an online library of the obtained structures, where these structures are freely available.

Employing these structures in molecular dynamics simulations, we investigated the interactions of MNPs with the antibiotic tetracycline and the corresponding binding energies. The results showed a good qualitative agreement with experimental data on binding affinities, and in vitro experiments on the absorption of the drug in the presence of MNPs. To uncover the environmental effects of MNPs, their interactions with biomolecules must be understood. The results presented here will include the interactions of these pollutants with lipid bilayers, proteins, and DNA. In case of lipid bilayers, we showed that the corona on the plastic has a decisive effect whether the MNP can cross a membrane. The obtained results indicated that these particles can cross the blood-brain barrier. In agreement, in toxicology experiments on mice only two hours after being fed with food containing environmentally relevant concentration of MNPs, plastic particles appear in the brain tissue. Simulations and quantum chemical calculations showed that MNPs can alter the secondary structure of proteins. Depending on the plastic compound, the relative energy between α-helix and β-sheet structures of the same protein can be shifted significantly. While polyethylene was found to stabilize the helix, nylon-6,6 was prone to change the peptide into a β-sheet, which may have severe physiological consequences. Similarly, upon interacting with polymer chains, DNA was found in molecular dynamics simulations to shift from the most common B form to its A conformation, which also raises alarming possibilities on the environmental effects of these materials.

Single-molecule mechanics of chemically modulated DNA

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ABSTRACT

Double-stranded (ds) DNA is the target of numerous chemical effects that modulate its structure and function. Single-molecule manipulation with optical tweezers allows us to uncover the mechanisms of these modulatory effects with unprecedented detail. Here we investigated the effect of hypermethylation and porphyrin binding to DNA.

Cytosine methylation is a key mechanism of epigenetic regulation and has long been suspected to alter the physical properties of DNA. We measured the methylation-induced nanomechanical changes in a DNA molecule with the sequence of a CpG island [1]. Contour length, bending rigidity and intrinsic stiffness decreased in hypermethylated dsDNA, pointing at structural compaction which may facilitate DNA packaging *in vivo*. Intriguingly, increased forces were required to convert hypermethylated dsDNA into an extended S-form configuration. The reduction of force hysteresis during mechanical relaxation indicated that methylation generates a barrier against strand unpeeling and melting-bubble formation.

TMPyP is a porphyrin capable of DNA binding and used in photodynamic therapy and G-quadruplex stabilization. We investigated how TMPyP influences DNA nanomechanics across wide ranges of TMPyP concentration, mechanical force, NaCl concentration and pulling rate [2]. TMPyP binding causes dsDNA lengthening, softening, a bi-phasic change in structural stability, and to an increase in ssDNA contour length. NaCl competes with the TMPyP-evoked nanomechanical changes.

Altogether, the chemically-induced changes in DNA nanomechanics may be used to tune DNA's structure and properties, hence control the wide array of DNA-dependent processes including replication, transcription, condensation and repair.

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Oral contributions

NMR for Colloids: Achievements and Pitfalls

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ABSTRACT

NMR has come a long way in the 80 years since its discovery. Its triumph began with the discovery of chemical shift; however, nuclear relaxation was always present - sometimes in the background, sometimes in focus. ^{1}H and ^{13}C NMR became essential tools in organic chemistry. The advent of superconducting magnets and the application of pulse techniques made it possible to characterize colloid-sized organic macromolecules and biomolecules. Applications in classical colloid chemistry began with the early recognition of the “disturbing effects” of Brownian motion or self-diffusion in relaxation measurements. From these experiments, a simple tool for determining particle size was developed. As with every simple experiment, this also led to oversimplification in the interpretation of results, as I will show in this lecture. Diffusion in porous systems can be measured, enabling the determination of pore size and liquid permeability.

In liquid-state NMR, the solid material-for example, the frozen state of a liquid-can be disregarded. Therefore, NMR is a simple tool for determining freezing and melting curves in porous systems. By applying the Gibbs-Thomson equation to freezing or melting point depressions, the surface-to-volume ratio can be determined; in the case of known pore geometry, the pore size distribution can be established. Under certain conditions, the pore shape can also be revealed.

The disadvantages of NMR are its high cost and expensive maintenance. A reasonable alternative is low-field NMR or NMR relaxometry, which uses a permanent magnet and detects only nuclear relaxation. In this case, the interaction between the liquid environment and colloids is measured. The advantages are low cost and cheap maintenance; the disadvantages are the indirect nature of the information and the less developed methodology.

In this lecture, I will present examples from both the bright and dark sides of liquid-state NMR applied on colloid systems.

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Self-diffusion and clustering phenomena in magnetically controlled ferrogranulate system

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ABSTRACT

Understanding the dynamics of ferrogranulates – mixtures of magnetic and non-magnetic particles under competing forces - sheds light on their self-assembly and transport properties. This work combines experimental studies with Langevin dynamics simulations to explore the interplay of magnetic forces, particle area fractions, and external out-of-plane magnetic inductions. High-speed vibration experiments capture the structural evolution of steel and glass beads, while simulations provide insights into the governing microscopic interactions.

Our findings reveal that increasing magnetic induction enhances individual particle mobility but suppresses collective clustering. Clusters form due to a balance between repulsive and magnetic forces, transitioning between distinct behaviors with changing induction strength. Furthermore, all analysis indicates normal diffusion for glass particles and single magnetic particles at high induction, while clustered particles exhibit sub-diffusive behavior due to magnetic interactions and crowding.

Through a novel linking of simulation temperature to experimental acceleration, we propose a scaling framework for diffusion and demonstrate deviations from classical models. These results illuminate the tunable nature of ferrogranulates and suggest future studies under dynamic or spatially varying magnetic inductions. Our work paves new paths for applying magnetic control in granular physics and related disciplines.

Budesonide-loaded liposomes for inhalation

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ABSTRACT

Liposomes are nano-scale drug carrier systems with the ability to improve several pharmacokinetic properties of the encapsulated drug. Our goal was to create budesonide-loaded small unilamellar liposomes with long-term shelf-life for inhalation in chronic inflammation-related conditions like asthma or COPD.

The liposomes (composed of 3 different phospholipids: DSPC, DPPC, and DMPC) were made by thin layer hydration technique and extrusion. Their basic physicochemical properties were determined: size distribution by dynamic light scattering, encapsulation efficacy by size-exclusion gel chromatography and HPLC, and phase-transition temperature by differential scanning calorimetry. The lamellarity of the liposomes was investigated by freeze-fracture technique and small-angle X-ray scattering. The possible chemical interactions between the components were evaluated by Fourier Transform Infrared Spectroscopy. We also checked the interaction of the liposomes with the EBC-1 human lung carcinoma cells. The freeze-drying method were optimized regarding the type and ratio of a cryoprotectant disaccharide and the amount of the encapsulated drug. The size distribution of the lyophilized powder was measured in a cascade impactor.

As a result, we were able to create budesonide-loaded liposomes with a hydrodynamic diameter of 120-140 nm. The encapsulation efficacy was around 87%, and the presence of the drug did not significantly affect the phase transition temperature.[1] Most of the vesicles were unilamellar but a small portion was bilamellar. No chemical reaction was detected between the components of our drug formulation. Our liposomes could get into the investigated lung cells and showed no cytotoxicity. For freeze-drying, a high ratio of trehalose and 10 m/m% budesonide was ideal.

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Electrohydrodynamics based Functional Fibers for Wireless Neuromodulation

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ABSTRACT

The significance of the overall fibrillar and porous nanoscale topography of the extracellular matrix in promoting essential cellular processes has led to consideration of biomaterials with nanofibrous features. Of the many methods for fabricating fibers with micrometer and nanometer diameters, electrohydrodyanmics (EHD) based spinning is simplest, most straightforward and cost-effective. This approach becomes intriguingly powerful when remarkable morphological features were combined with unique chemical, physical, or mechanical functionalisation with ease and control. [1,2]

Alongside the widely studied pathways of biochemical regulation by chemokines, cytokines and growth factors, one often overlooked but significant influence over the behavior of biological systems is electrical signaling. Voltage gradients among all somatic cells (not just excitable nerve and muscle) control cell behavior, and the ionic coupling of cells into networks via electrochemical synapses allows them to implement tissue-level patterning decisions, which is called developmental bioelectricity. Electrical modulation is therefore a potential target for many new therapies for a range of diseases and biological functions. Our current research focuses on advancing EHD technologies to explore multi-dimensional nano-biointerfaces that synergise the nano structural induction and the bioelectrical/biochemical signalling to affect cellular behaviours, for biomedical applications in neuromodulation and tissue engineering[3-5].

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Tough gel based ionotronics for flexible electronics

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ABSTRACT

Gels including hydrogel, organogel, and ionogels have aroused much attention in flexible electronics. Diversified demands put forward comprehensive requirements for multifunction, intelligence and mechanical properties of gel based ionotronics. Given the applications of gel based ionotronics in diverse scenarios, we have developed a series of strategies to achieve ionic conductive hydrogels, organogels, and ionogels with high mechanical properties (high strength, toughness, impact resistance, puncture resistance, rapidly self-recoverable). Furthermore, the applications of these tough gel based ionotronics in intelligent flexible electronics, such as continuous passive motion system, underwater therapy exercise monitoring, and human-machine interaction systems were explored.

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Development of Electrospun Wound Healing Matrices Using Metal Nanoparticles

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ABSTRACT

Combating multidrug-resistant bacteria is an increasing challenge in healthcare, especially in the treatment of slow-healing wounds such as diabetic ulcers. Since traditional antibiotics are often ineffective, alternative antimicrobials are needed. [1,2] Metal oxide nanoparticles (MeNPs) are promising candidates due to their strong antibacterial activity and lower tendency to induce resistance. However, their potential cytotoxicity makes safe use in living tissues challenging. [3]

The aim of this research was to create a wound dressing by incorporating MeNPs into a biocompatible and biodegradable polymer matrix prepared by electrospinning. A key challenge was to disperse the nanoparticles in volatile organic solvents compatible with electrostatic fiber formation.

Oleic acid-stabilized magnetite nanoparticles (MNPs) were synthesized, and ultrasonically dispersed in the polymer solution. Zinc-oxide nanoparticles (ZnONPs) were prepared in dimethyl sulfoxide, followed by optimization of precursor materials, reaction, and centrifugation parameters. DLS was used to determine the hydrodynamic diameter and polydispersity index of ZnONPs, and UV-Vis spectrophotometry confirmed the presence of both nanoparticle types.

Electrospinning was successfully used to produce fibrous meshes from the MeNP-containing polymer solutions, confirmed by SEM. EDX demonstrated successful nanoparticle incorporation, and FTIR monitored the structures of the materials. Antibacterial tests on four standard strains showed enhanced activity in ZnONP-loaded scaffolds compared to controls. Mechanical properties were evaluated using a tensile testing system.

These findings demonstrate the potential of PSI-based nanofibrous materials containing MNPs and ZnONPs as antibacterial wound dressings. Future work will include cytotoxicity assays on fibroblast cells and advanced structural characterization using TEM and SAXS.

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ACKNOWLEDGEMENTS

This research was supported by NKFIH FK 137749, TKP2021-EGA-23 research grants and the Semmelweis Travel Grant.

Microplastics and heavy metals in sewage sludge and the effect of their co-occurrence on *Pseudomonas aeruginosa*

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ABSTRACT

Sewage sludge originating from municipal wastewater treatment plants (WWTPs) is frequently applied as an agricultural fertilizer due to its rich nutrient content; however, it also carries various contaminants, including heavy metals, microplastics (MPs), and can be considered as a hot spot for antibiotic-resistant bacteria (ARBs) [1]. In this study, we explored the simultaneous presence and potential interactions of these pollutants in sludge samples collected from eight wastewater treatment plants across Hungary. MP concentrations were measured using both pyrolysis gas chromatography/mass spectrometry (Py-GCMS) and Fourier-transform infrared spectroscopy (FTIR) [2], revealing the average values of particles per gram of dry weight (dw). Based on our findings, the approximate volume of MPs that are possibly introduced into Hungarian agricultural soils through sludge application is significant. According to our results, all sludge samples contained heavy metals, while antibiotic resistant strains of *Pseudomonas aeruginosa*, a human pathogen, were detected in seven out of eight samples. The concentration of heavy metals often stayed at sublethal levels for the isolated strains [3], creating conditions that could trigger resistance development. Moreover, MPs act as carriers by adsorbing metals and enhancing the formation of biofilms, which provides adequate circumstances for antibiotic resistant bacteria [4] such as *P. aeruginosa*. Our results underscore the urgency of updating regulatory frameworks and enforcing more rigorous monitoring of sludge composition to limit environmental pollution and the spread of resistant microorganisms and resistance genes.

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Swelling and structure of biodegradable crosslinked polyurethanes by NMR

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ABSTRACT

Biocompatible and biodegradable polymers are popular nowadays due to the growing demand of medicine, pharmacy, and environmental protection. Polyurethane-based polymers are appropriate for this purpose with e.g. sucrose moieties in the crosslinking points and with their outstanding physical and mechanical properties. Crosslinked polymer networks are usually tested by their thermal, mechanical, and swelling properties; however, liquid phase nuclear magnetic resonance (NMR) spectroscopy is an appropriate complementary technique, being able to give direct information about the details of structural changes during swelling.[1]

In this study, we applied various NMR methods to describe the interaction of biodegradable polyurethane polymers crosslinked to different extent with DMSO and water, a well and less swelling liquid phase, respectively. We separated the rigid and mobile domains in the amorphous part of the plasticized polymer through their relaxation properties from the swelling liquid among the polymer chains. The swelling process can be followed by the transverse relaxation of the domains, among which the relaxation rates of the swelling liquid correlated with the degree of swelling due to the size change of the confinements. This offers a novel approach to the description of swelling kinetics and mechanism. We observed second-order kinetics in DMSO, and concluded the interpretation of the swelling process on the molecular level. The macroscopic structural differences were further detailed by the diffusion properties of the swelling liquid, which were influenced by the joint effect of the crosslink density and the amount of dangling chain ends. The size change and the geometry of the liquid confinements were studied by NMR cryoporometry on the nanoscale.[2]

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Co-immobilization of protease enzyme and molecular antioxidant on anionic clays

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ABSTRACT

The synchronized operation of antioxidants and enzymes is necessary for the proper functioning of living organisms and for various industrial processes. Antioxidants prevent or interrupt harmful oxidation reactions caused by reactive oxygen species (ROS) and thus anticipate oxidative stress [1]. Enzymes, on the other hand, accelerate biochemical reactions through their specific (e.g. proteolytic) catalytic functions [2]. However, these biomolecules can be susceptible to several environmental factors (e.g. sensitivity to temperature, pH, low water solubility), which can then lead to the loss of their activity under inadequate conditions. These drawbacks can usually be overcome by their immobilization using appropriate methods. Layered double hydroxides (LDHs) are biocompatible, chemically and mechanically stable materials that are therefore suitable carrier materials [3]. The aim of our study was to immobilize tannic acid (TA) and papain (PPN) on LDH nanoparticles in order to enhance their stability and facilitate their combined use advantageous in food industry, for instance. TA and PPN were immobilized on the surface of the LDH nanoparticles by electrostatic interactions. The adsorption of TA resulted in a charge reversal of the originally positively charged LDH particles, while PPN was immobilized on the negatively charged LDH/TA nanocomposites. The characteristic peaks of TA and PPN in the Raman spectrum of LDH/TA/PPN and the results of the Bradford assay confirmed the successful immobilization of TA and PPN on the surface of the nanoparticles. The composite had significant antioxidant and proteolytic activity after binding of the two molecules. In conclusion, TA and PPN were unambiguously immobilized on LDH nanoparticles, which conferred antioxidant and proteolytic activity to the LDH/TA/PPN composite. Moreover, the resulting composite possessed high colloidal stability, which makes the nanocomposite a promising material for use in industrial processes where the simultaneous application of the two biomolecules would be advantageous in heterogeneous systems.

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Visible Light Photocatalytic-Adsorption Effect of Recyclable Industrial Waste

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ABSTRACT

Removal of the contaminants/organic dye pollutants from wastewater provides a relevant global challenge. In this work the photodegradation of organic pollutants was aimed to realise by means of a very dangerous, toxic industrial waste, the red mud.[1] Beside of the environmental aspect, the economic respect was also considered by recycling of an industrial waste and using visible region for photodegradation instead of generally applied ultraviolet light. The photocatalytic properties of red mud (RM) were tested in the solution of analytical indicators used as model agents (methylene blue, Congo red, and crystal violet) and real organic pollutants (cortisone and corticosterone). The mechanism of degradation effect (photocatalytic effect and/or adsorption) has been clarified. The degradation effect of RM was detected using ultraviolet-visible (UV-VIS) and fluorescence spectroscopies. The connections between pollutants and red mud were investigated by infrared spectroscopy (FTIR).

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From Hydrogen to Fluorine: Structural and Dynamic Consequences in Alcohols Explored by MD and SWAXS

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ABSTRACT

Fluorinated alcohols, though not typical PFAS – best known as persistent fluorinated compounds of environmental concern – can serve as practical molecular models for studying fluorination effects on molecular organization and intermolecular interactions. In this study, small- and wide-angle X-ray scattering (SWAXS) and molecular dynamics (MD) simulations are combined to study their structural and dynamical properties and rheological behavior. The complemented- system approach [1,2] is used to calculate theoretical SWAXS intensities from simulation results, allowing for direct comparison with experiment and validation of molecular models. The study proceeds in two steps. First, we compare three linear trifluoromethyl alcohols with their hydrogenated analogs. This shows that fluorination leads to a suppression of the OH-related inner scattering peak [3] and to the emergence of CF_3-dominated segmental organization. Second, we evaluate how increasing fluorination and altered substitution patterns in fluorinated butanol affect the liquid structure. We observe clear correlations between the degree of fluorination and the positions of the scattering peaks. The MD simulations also provide transport and rheological parameters — self-diffusion coefficients and zero-shear viscosities — that vary systematically with molecular structure. Fluorinated alcohols thus serve as effective models for studying the behavior of PFAS and provide insight into how subtle molecular changes modulate supramolecular organization and dynamic properties. These results support future studies of PFAS transport and interactions in more complex systems.

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Polymers at the air-water interface

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ABSTRACT

Thin polymer films based on polymer blends can be used as coatings with tunable properties. Such films can be created with the Langmuir film method: polymers are deposited on water controlling their density by compression, potentially cross-linked to obtain networks, and subsequently transferred onto a solid substrate resulting in stable thin films. As a first step to design such films, the miscibility properties of non-cross-linked polymer blends must be understood. In this work, we focus on understanding the miscibility properties of amphiphilic poly(ethylene glycol)-poly(propylene glycol)-poly(ethylene glycol) triblock copolymer and predominantly hydrophobic poly(dimethylsiloxane) (PDMS). We analyzed surface pressure-area isotherms to determine the phase transitions of the blends and used Brewster angle microscopy (BAM) to understand the mixing behavior at the interface. We combined these results to build a surface pressure-composition phase diagram (figure 1) where orange points represent the start of a phase separation observed with BAM and squares the phase transitions obtained from pressure-area isotherms. To connect the phase diagram with molecular level information, sum frequency generation (SFG) spectroscopy was performed. With this method the vibrational spectrum of the interface can be obtained. In the CH spectral region, we monitored the symmetrical CH stretching vibrations of the pure polymers. We conclude from the peak amplitudes that in the miscibility region the amplitudes increase linearly and they level when the system is de-phased.

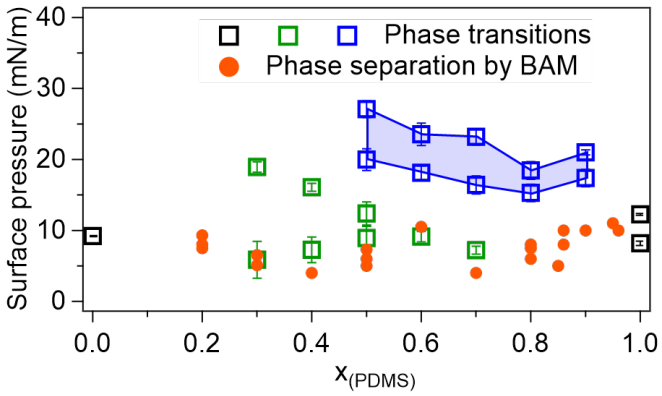

Figure 1: Surface pressure-composition phase diagram. The area marked with blue corresponds to the co-existence of two phases.

3D plasma assisted adsorptive removal of organic pollutants from water by porous carbon

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ABSTRACT

Porous carbon materials, extensively used in water treatment industry for their excellent adsorption properties, show considerable water purification potential while often being converted to hazardous solid waste themselves.

The 3D plasma generated by electric discharges in water and at air/water interface and UV light emitted by the plasma create a strongly oxidising environment potentially able to destroy organic chemicals regardless of their composition and structure. In addition, the strongly oxidising environment created in the plasma reactor should be able to destroy the biological hazards and ensure the elimination of the threat of transmitting waterborne diseases.

Per- and polyfluoroalkyl substances (PFAS) are a large class of thousands of synthetic chemicals that are used throughout society. However, they are increasingly detected as environmental pollutants and some have negative effects on human health. Owing to their carbon-fluorine bonds they resist degradation when used and also in the environment. The most efficient approach should be to convert them ideally into inorganic (mineral) products such as CO_2, water, fluoride anion, etc.

We combined the use of carbon adsorption and nonthermal atmospheric plasma treatment of water contaminated with model aqueous solutions of methylene blue and PFAS. The alteration of the adsorbent was also followed. The results of their collective use showed a synergistic effect in efficient removal of these contaminants.

ACKNOWLEDGEMENTS

This research was performed within the frame of the EU project CLEANWATER (HORIZON-MSCA-2022-SE-01 #101131382). This work is also part of the projects BME-EGA-02 supported by the Ministry of Culture and Innovation of Hungary from the NRDI Fund, under the TKP2021 funding scheme.

Molecular Dynamics simulation of adsorption and aggregation of therapeutic antibody fragments at water-oil interfaces

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ABSTRACT

Monoclonal antibodies (mAbs) are widely employed in targeted therapies for various diseases; however, their stability and physicochemical properties present significant challenges in biopharmaceutical formulations. A primary concern arises from structural alterations induced by interactions of the mAbs with oil-water interfaces and surfaces during storage, [1] which can lead to protein aggregation and a consequent loss of therapeutic efficacy. [2] Understanding the molecular mechanisms governing mAb adsorption is critical for developing strategies to mitigate interface-induced destabilization. While experimental techniques such as neutron reflectivity have been utilized to investigate adsorption, the interpretation of the results relies on microscopic models that require assumptions regarding the thickness of mAb monolayers and mAbs orientation. Here, we employ molecular dynamics (MD) simulations and coarse-grained force fields to probe the adsorption and aggregation behaviour of mAbs at liquid-liquid interfaces.

We employed the Martini 3 force field to investigate the adsorption and aggregation behaviour of fragments of monoclonal antibodies at the water–hexadecane interfaces. Our simulations reveal that specific amino acids play a key role in fragment adsorption, acting as interfacial “hot spots.” These findings provide insights into the molecular mechanisms governing antibody behaviour at interfaces, contributing to the rational design of protein-based formulations and biophysical studies.

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S100B chaperone modulates phenol-soluble modulin amyloid formation in *Staphylococcus aureus biofilm*

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ABSTRACT

Phenol-soluble modulins (PSMs) are key peptide virulence factors critical to the pathogenicity of *Staphylococcus aureus* in both community-associated and hospital-associated infections. Beyond their well-characterized cytotoxic effects, PSMs exhibit a pronounced propensity to self-assemble into fibrillar structures, a process likely mediated by the adoption of amphipathic conformations [1]. Meanwhile, the S100 protein family, characterized by calcium-binding EF-hand motifs, serves as key mediators in calcium-dependent signaling and inflammatory responses. These proteins exhibit direct antimicrobial activity against various pathogens, including those implicated in skin infections, and modulate immune reactions during bacterial invasion [2]. Despite growing insights into the functions of S100 proteins and PSMs, the interplay between S100 proteins and PSM-mediated amyloid aggregation—particularly its implications for biofilm formation and virulence—remains poorly understood. In this study, we investigate how S100B, a highly abundant proinflammatory S100 protein, influences the aggregation behavior of PSM peptides (PSMα1, PSMα3, and PSMβ1). Our findings reveal that S100B differentially modulates PSM aggregation, with a pronounced inhibition effect on PSMα3, an atypical α-sheet structures post-aggregation [3]. These results provide new insights into the potential regulatory role of S100 proteins in S. aureus biofilm dynamics and pathogenicity.

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Fabrication, Degradation Dynamics and Mechanical Integrity of Advanced Composite Electrospun Meshes

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ABSTRACT

INTRODUCTION:

Tissue integration is a vital yet complex aspect of regenerative medicine. When implants fail to support adequate cell adhesion, migration, or infiltration, the immune system often responds by forming a fibrous capsule, isolating the material and compromising its function. To improve integration, researchers have increasingly explored polymer blends and composites. Polycaprolactone (PCL) and polylactic acid (PLA) are commonly used in biomedical settings due to their biocompatibility and stability, though they suffer from hydrophobicity, poor cell attachment, and slow degradation. Polysuccinimide (PSI), a biodegradable and biocompatible polymer with excellent cell adhesion properties, offers a promising complement. Combining PSI with PCL or PLA may overcome individual limitations and enhance tissue compatibility.

OBJECTIVES:

This project aimed to develop and evaluate electrospun meshes composed of PSI blended with PCL and PLA, respectively.

MATERIALS AND METHODS:

Electrospun meshes were fabricated using PSI/PLA and PSI/PCL blends. These were then subjected to structural, chemical, and mechanical assessments.

RESULTS:

Microscopic analysis revealed uniform fibers without structural defects. ATR-FTIR spectroscopy confirmed the presence of both polymers in each mesh. The average fiber diameter was 650 nm for PSI/PLA and 600 nm for PSI/PCL. Specific loading capacity was higher in PSI/PCL (0.250 Nm^2/g) compared to PSI/PLA (0.061 Nm^2/g). Both meshes showed progressive weight loss and a corresponding reduction in tensile strength during the degradation process.

CONCLUSION:

The PSI/PLA and PSI/PCL electrospun meshes displayed favorable structural and degradation characteristics, making them strong candidates for tissue engineering applications. PSI/PCL, in particular, demonstrated superior mechanical properties, supporting its potential use in load-bearing or mechanically sensitive regenerative contexts.

Swimming nanorobots for targeted therapy in glioblastoma treatment

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ABSTRACT

Glioblastoma remains a substantial obstacle in therapy since the blood-brain barrier (BBB) and tumor microenvironment (TME) severely prevent the access of most exogenous therapeutic agents to the central nervous system. To address this, we develop a Trojan horse-inspired enzymatic nanobot-in-neutrobot system (Trojanbot) to greatly enhance targeted GBM therapy. Trojanbots traverse the BBB by leveraging positive chemotaxis in response to tumor-derived chemokine gradients, after which the released catalase-driven nanobots (CatNbot) undergo directional movement along the H_2O_2 gradients in TME, facilitating deep tumor penetration. This strategy advances GBM therapy and shows broad potential for other cancers and neurological diseases. Its dual-targeting design enables adaptation to complex microenvironments, supporting applications in precision medicine.

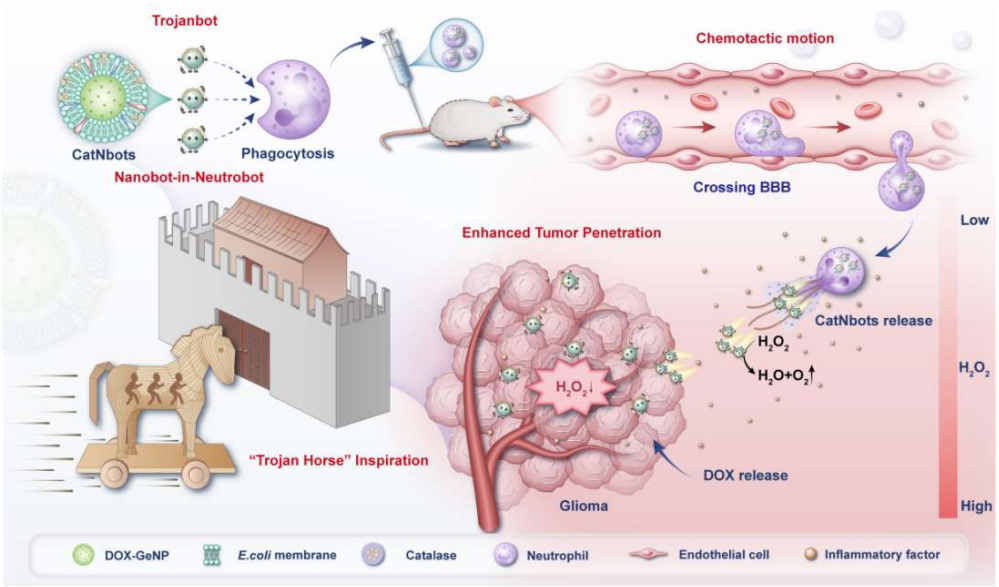

Figure. 1 Schematic illustration of the enzymatic Nanobot-in-Neutrobot system.

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From powder to beads: insights into an imine-linked triazine porous organic polymer for the remediation of fluoroquinolone antibiotics from water

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ABSTRACT

Water pollution, particularly with antibiotics, contributes to the induction and spread of antimicrobial resistance, which are two of the main problems plaguing humanity [1]. Therefore, simple strategies must be developed to promote their efficient remediation. This communication describes an imine-linked triazine porous organic polymer (IT-POP, Fig. 1A) as a novel highly stable micrometer-sized advanced adsorbent material, containing hydroxyl, as well as carboxyl groups (0.43 mmol g^{-1}) that after deprotonation make IT-POP negatively charged (isoelectric point at pH = 4.7) and effective for ciprofloxacin (CPX) and levofloxacin (LVX) removal (efficiencies up to 99% (Fig. 1B) and maximum sorption capacities up to 0.34 mmol g^{-1}). To up-scale application, IT-POP-containing starch-alginate beads (Fig. 1C) were developed, and those with 10 w/w% of IT-POP proved to be an efficient, economical and processable solution for day-to-day application, since the removal capacities of CPX and LVX only decreased by 2 fold when the mass of IT-POP functional material decreased 10×, meaning a 5× increase in performance after its incorporation into the polysaccharide matrix. The powder and the beads also efficiently removed 6 out of 7 antibiotics mixed at µM scale, showing residual affinity for amoxicillin and greater selectivity for sulfonamides and fluoroquinolones (CPX and LVX). Furthermore, a comparison between batch and continuous flow adsorption studies was made, proving again the high potential of the materials for the decontamination of antibiotic-containing effluents.

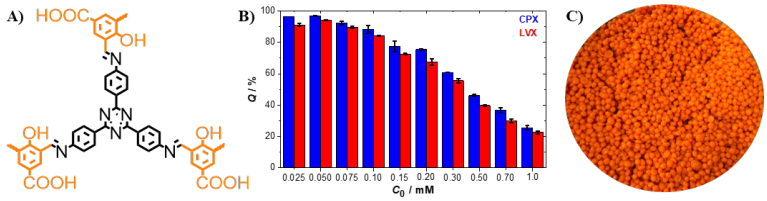

Fig 1. A) Chemical structure of IT-POP; **B)** Effect of the initial concentration on the removal efficiencies of CPX and LVX by IT-POP; **C)** Photograph of IT-POP-containing starch-alginate beads.

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Acknowledgements: To Coimbra Chemistry Centre (CQC-IMS), supported by FCT (Portugal) through the programs UIDB/00313/2025 & UIDP/00313/2025. P.M.C. Matias also thanks FCT for the PhD Grant 2022.12425.BD. This study was also financed, in part, by FAPESP (Brazil) through processes #2022/11133-0, #2023/11783-8 and #2020/13703-3.

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Extracellular vesicles detection via surface enhanced IR spectroscopy using plasmonic gold nanoparticles

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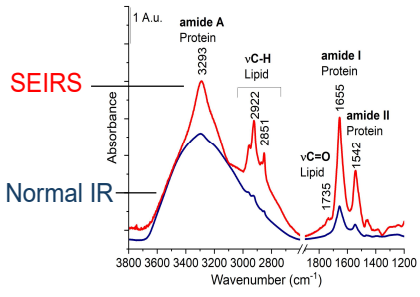
Extracellular vesicles (EVs), spontaneously released by cells, play an important role in intercellular communication. Due to their special size and composition (lipid bilayer-bounded nanosystems, usually smaller than 200 nm, containing both proteins and RNAs), EVs potentially can be used in diagnostics as “next-generation” biomarkers. Infrared (IR) spectroscopy, especially attenuated total reflection (ATR), is a rapidly emerging label-free tool for molecular profiling of EVs. The relatively low number of vesicles in biological fluids (~10^{10} particle/mL) and the complex content of the EVs milieu (protein aggregates, lipoproteins, buffer molecules), however, might result in poor signal-to-noise ratio in the IR analysis of EVs. Exploiting the increment of the electromagnetic field at the surface of plasmonic nanomaterials, surface-enhanced infrared spectroscopy (SEIRS) might provide an amplification of characteristic IR signals of EV samples .

Negatively charged citrate-capped and positively charged cysteamine-capped gold nanoparticles with around 10 nm diameter were synthesized and tested with blood-derived EVs [1]. Since the interaction between EVs and AuNPs is a key factor in obtaining SEIRS phenomenon, changes in plasmonic properties and possible aggregation of AuNPs were investigated by UV-Vis spectroscopy, dynamic light scattering (DLS) and freeze-fracture transmission electron microscopy (FF-TEM).

The positively charged cysteamine-capped AuNPs proved to be more advantageous for SEIRS measurements:



i) higher enhancement was achieved for both lipid- and protein-related IR bands; ii) unlike citrate-capped AuNPs, there is no spectral interference with amide I and amide II protein bands. Fine-tuning the surface properties of gold colloids can further lead to selective enhancement of EVs' infrared signals. This work not only advances methodologies for EV characterization but also contributes to the field of SEIRS.

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Synthesis and properties of hydrogel fibers

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ABSTRACT

Gel fiber based membranes have a unique structure mimicking the structure of native soft tissues. As such, they can be used as materials for cell cultivation and in tissue regeneration. However, there is a constant need for new methods for the preparations of such materials, since there are no general strategies for their synthesis. The use of water soluble polymers in the synthesis of implants using electrospinning is inappropriate because of their fast dissolution in biological fluids. By utilizing reactive electrospinning, chemically crosslinked gel fibers can be synthesized, which, without enzymatic or chemical degradation, will not dissolve in physiological conditions. Polysuccinimide (PSI) is the anhydrous form of poly(aspartic acid), which is a biodegradable and biocompatible artificial polypeptide. Polysuccinimide can transform into poly(aspartic acid) above pH 7.4 and also in the body [1]. Other advantage of this polymer system is that polysuccinimide can be easily modified with primary amines and thus a wide variety of polysuccinimides and poly(aspartic acids) can be synthesized. Based on this flexibility, different techniques were developed to make crosslinks between the PSI chains inside the fibers: after placing free thiol groups as side groups on the polymer, thiol oxidation crosslinking by air during electrospinning [1,2]; immersion of electrospun PSI fiber mats into a diamine crosslinker solution to post-electrospinning crosslink the fibers [2]; using coaxial electrospinning, where the crosslinker was in the core and the PSI solution was in the shell [3]; and using non-equilibrium low pressure air plasma in allylamine-modified polysuccinimide fibers [4]. After the hydrolysis into the poly(aspartic acid) based hydrogels, the membranes show pH dependent swelling properties which were also investigated. These strategies can be applied to other polymer systems as well..

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Influence of Crowders and Ligands on the Polymeric Properties of G-Quadruplex Multimers

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ABSTRACT

G-quadruplexes (G4s) are non-canonical DNA structures formed by guanine-rich oligonucleotides [1]. They are abundant in higher eukaryotic genomes and particularly concentrated in telomeric regions, constituting up to 25% of all DNA G4s [2]. Single-stranded telomeric overhang sequences (ssTELs) can fold into various multimeric G4 configurations with distinct biological roles and interest as potential drug targets [3]. Most prominently, G4s have been shown to inhibit telomerase and HIV integrase, which opens the possibility for specific G4-stabilizing compounds to be utilized as anticancer or antiviral medications [4].

Many ligands have been identified to interact with ssTELs to stabilize G4 monomers [5]. Stabilization of ssTELs in cancer cells has been associated with apoptosis [6]. However, ligand effects on the properties of G4 multimers and the mechanisms underlying telomerase inhibition remain unclear. Large-scale, long-timescale computational studies are necessary to address critical gaps in understanding G4 behavior in crowded and non-crowded environments.

Using a novel coarse-grained G4 model and molecular dynamics simulations, we study polymeric properties of long telomeric G4 multimers and their modulation by various ligand molecules, both with and without crowders. Our approach is validated against in vitro experiments, demonstrating that long G4 multimers exhibit flexibility akin to polymers in good solvents. In crowded environments, G4 multimers show increased coiling propensity and reduced chain stiffness. Additionally, we demonstrate, in silico, a novel type of ligands we call poly-ligands, that intercalate more effectively into G4 multimers compared to their non-poly counterparts, offering new ways to manipulate the polymeric properties of G4 multimers.

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Relaxivity properties of paramagnetic metal ion complexes with polymers synthesized from smaller building blocks

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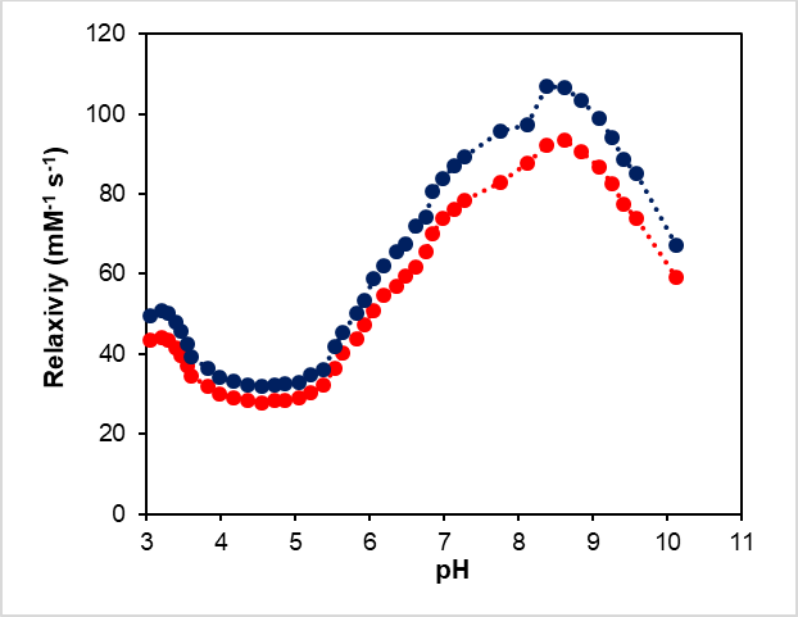
ABSTRACT

The slow tumbling motion of macromolecular paramagnetic metal complexes can be used advantageously to shorten the relaxivity time of water protons. This shortening effect depends on many parameters, including the nature of the metal ion, the number of water molecules coordinated to, the ligand to metal ratio, and the pH of the solution among other factors. To depart from the usual procedure consisting in the functionalization of polymer platforms with well-known chelators, we synthesized smaller building blocks using aminocarboxylic acid derivatives of unsaturated compounds (functionalized monomers) and used them as building blocks to yield chelating polymers. This way, an additional degree of freedom was gained by combining the type and quantity of the building block(s) incorporated into the polymer, resulting in different relaxivity profiles as a function of the pH. This dependence can be a valuable tool to induce magnetic contrast enhancement in different environments.



Polysuccinimide-based electrospun scaffolds loaded with different salts for potential use in wound dressings

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ABSTRACT

Although silver ions are commonly used in antibacterial agents for therapeutic purposes, they are associated with significant environmental impact and, in some cases, undesired immune responses. As a result, their use in medicine is gradually declining, with other antibacterial ions emerging as promising alternatives.

Our research aims to create a bicomponent polymer scaffold by electrospinning, which contains zinc and strontium salts in addition to the polymer, which, according to the literature, has antibacterial properties. If such a new type of biocompatible wound dressing could be created, it would be a mechanical barrier and have antibacterial activity against microorganisms.

Several experiments have been conducted to optimize the physicochemical, mechanical, and biological properties of the scaffolds developed for application as wound dressings. The first step was synthesizing the polysuccinimide (PSI) polymer, mixing it with the selected inorganic salts in dimethylformamide, and optimizing the electrostatic fiber formation parameters. The inorganic salts used in the experiments were zinc-acetate and strontium-nitrate. Next, the chemical and mechanical properties of the complete polymer networks were investigated by FTIR spectroscopy, SEM images, and their mechanical behavior through specific load capacity, elongation at breakpoint, and Young's modulus values. In the next step, we performed dissolution tests to examine whether the salts could dissolve from the scaffold and exert their antibacterial effect. After that, antibacterial activity tests were performed on four application-relevant bacterial species. The next step was determining if the polymer scaffolds with the salts have cytotoxic activity against human tumor and fibroblast cells. Because these fibrous structures will be used as wound dressing, they must interact with the human cells.

We did further research to combine the two salts' advantageous properties. Coaxial fibers are nanofibers that have a core and a shell layer. We aim to make an inner core layer that contains two salts and PSI, and an outer shell layer that includes the neat PSI to get a more extended dissolution profile. First, the coaxial electrospinning and mechanical characterization of the coaxial fibers have been optimized.

ACKNOWLEDGEMENTS

This research was supported by NKFIH FK 137749, TKP2021-EGA-23 research grants and the Semmelweis Travel Grant.

Quantifying Biofilm Formation on Different Plastic Surfaces

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ABSTRACT

Biofilm formation on plastic surfaces presents significant challenges across environmental, industrial, and healthcare sectors. Plastics such as polystyrene (PS), polylactic acid (PLA), polyethylene (PE), polypropylene (PP), polyethylene terephthalate (PET), and polyvinyl chloride (PVC) are extensively used and often exposed to microbial colonization. In healthcare, biofilms on medical devices can lead to persistent infections and increase antimicrobial resistance [1,2], while in food processing and manufacturing, they contribute to hygiene problems and economic losses [3]. Plastic material types can support or resist microbial attachment depending on their physicochemical surface properties [4]. Thus, understanding the extent to which different plastic types promote or inhibit biofilm formation is crucial for both public health and material safety. Among microbial colonizers, *Pseudomonas aeruginosa* is a particularly relevant model organism due to its role as an opportunistic pathogen capable of forming resilient, antibiotic-tolerant biofilms [5].

This study aimed to compare biofilm formation on various plastic surfaces using a standardized and quantitative approach. We initially applied tetrazolium salt based (MTT) assay, which quantifies the metabolic activity of viable biofilm-forming cells. The MTT method produced robust, reproducible, and quantitative data across all plastic types tested.

Our findings indicate that biofilm formation varied among polymer surfaces, with *P. aeruginosa* forming the most metabolically active biofilms on PS and LDPE, and the least on PVC and PET. These results suggest that the nature of the plastic surface plays a key role in supporting microbial colonization.

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Water Pollution Mitigation by Removal of Local Anesthetics via Liquid-phase Adsorption on Graphene Oxide

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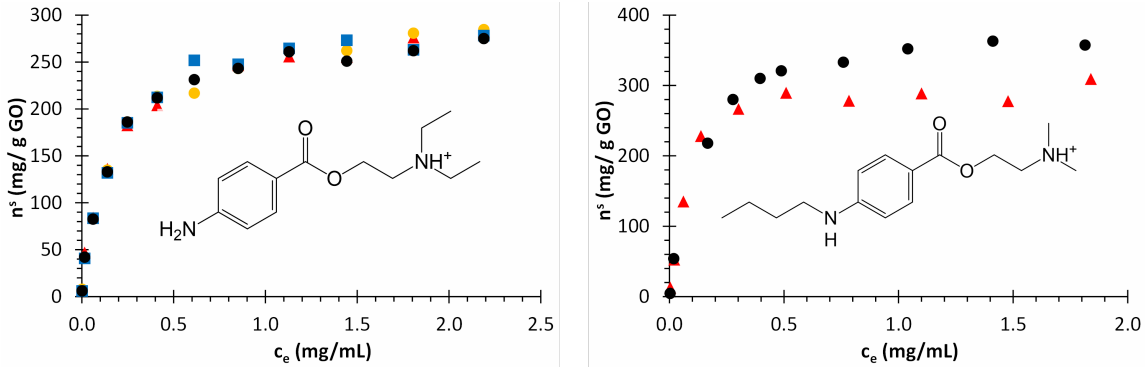
ABSTRACT

Pharmaceutical pollutants, especially local anesthetics, have been identified in natural waters[1], raising alarm over water quality and public health.

This study addresses the challenge of removing anesthetic compounds such as benzocaine, procaine, lidocaine, and tetracaine from aqueous solutions. Layered graphene oxide (GO) was utilized as an adsorbent due to its large specific surface area and ion-exchange capability[2].

Adsorption experiments quantified the interaction between GO and selected anesthetics, and changes in solution concentration were analyzed using photometric methods. Zeta potential and XRD measurements supported the findings. Experimental results showed that GO effectively adsorbed procaine and tetracaine (~290-350 mg /g GO), while lidocaine showed minimal adsorption and benzocaine showed none. Adsorption mechanisms were found to depend on the ionization state of the compounds and the physicochemical properties of the solution. This research demonstrates the potential of graphene oxide as an efficient solution for mitigating water pollution caused by pharmaceutical contaminants.



Adsorption isotherms of the “caine” drugs (left lidocaine, right tetracaine, T=298 K, I=10 mM NaCl, pH=7.4)

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Host–Guest Chemistry of β-Cyclodextrin with Platinum(II) Drugs: Inclusion Complex Formation and Cytotoxic Profiles

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ABSTRACT

Cancer's global impact emphasizes the need for improved chemotherapeutic agents. Since cisplatin's clinical introduction in the 1970s, efforts have aimed at developing metallodrugs with greater efficacy and lower side effects and acquired resistance. Recently, cyclodextrin-based inclusion complexes have gained attention for enhancing drug stability, solubility, targeting, and reducing toxicity and resistance. [1] Although platinum(II)-based drugs are well studied and clinically applied, their use is often hindered by poor aqueous solubility and severe resistance upon administration. [2] Drug-CD inclusion complexes are therefore a promising, yet underexplored, approach to overcoming these limitations. In this study, five new β-CD–Pt(II) inclusion complexes were prepared using commercial β-CD and its cationic (monoamino-β-CD) and anionic (succinyl-β-CD) derivatives. Cisplatin (*cis*-$Pt(NH_3)_2Cl_2$) and the dinuclear Pt(II) complex Pt_2Put_2 (Put=putrescine=$(CH_2)_4(NH_2)_2$), were selected as model drugs. The corresponding inclusion complexes were characterized by TGA, elemental analysis, NMR and vibrational spectroscopy. Cell viability assays (in triple negative breast cancer cell lines – MDA-MB-231) and evaluation of metabolic impact by microRaman and microFTIR evidenced an improved anticancer activity of the drugs upon CD inclusion, underscoring the potential of CD host–guest systems in advancing cytostatic drug formulations.

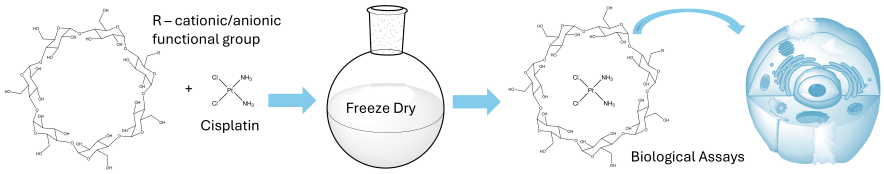

Fig. 1. Schematic illustration of inclusion complex formation and subsequent biological assays.

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Acknowledgements: QFM-LAQV/Requimte is supported by national funds through FCT – Foundation for Science and Technology, I.P., under the project UIDB/00070/2020. J.A.V.S. acknowledge FCT (grant UIDB/00070/2020) for financial support.

Molecular dynamics simulations of Magneto-active elastomers

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ABSTRACT

Magneto-active elastomers (MAEs)[1-2], or magnetorheological elastomers (MREs), have gained interest for their ability to change mechanical properties using low-energy magnetic fields - one can change the material stiffness, surface roughness and shape. This, coupled with clever engineering, enables innovative designs, especially in the field of soft robotics.

MAEs consist of an elastic matrix with embedded magnetic micro- or nanoparticles, magnetically either hard (HMPs) or soft (SMPs). For high concentrations of magnetic particles, the system can be modeled as a complex arrangement of randomly bonded HMPs[3] - through springs. As a consequence, the model cannot capture the incompressibility of MAEs.

We aim to address this issue and implement in ESPResSo[4] the necessary features for accurate MD simulations of MAEs. This will enable us to study the magneto-mechanical response of bulk and free surface MAE. We focus on the impact of SMP on the surface relief of a MAE layer. We provide a critical comparison between HMP- and SMP-based MAE for optimizing controllable wetting properties of functionalized surfaces.

Figure 1. *Simulation snapshot of MAE [5]. The surface roughness is magnetic field controlled.*

Keywords: magneto-active elastomers, magnetic soft matter, soft robotics

Acknowledgements: This research is funded by the EU's Horizon Europe research and innovation programme Doctoral Network MAESTRI (grant agreement No. 101119614).

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Liposomal formulations of flavonoids

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ABSTRACT

The creation of liposomal formulations in the pharmaceutical industry has gained great significance recently. Due to the importance of these systems, our research group started designing liposomal formulations a few years ago [1, 2] and as a continuation of the work, we planned to carry out the encapsulation of drug molecules from the family of flavonoids (the strongly hydrophobic quercetin and its more water-soluble derivative, rutin) into these kinds of colloidal particles. Also, liposomal formulation of these molecules does not exist in the pharmaceutical industry yet, which is a further motivation of the work.

Since the characteristics of the liposomal formulations strongly depend on the preparation method, 3 different ways (the thin layer hydration, the solvent injection and the microfluidic method) of creating particles were investigated and evaluated based on numerous aspects. According to our results, in the case of quercetin ~150 nm liposomes were fabricated with both the thin layer hydration and the solvent injection method as well, with ~95% and ~28% encapsulation efficiency, respectively and relatively good stability over 2 weeks. Also, greater retention of quercetin was achieved in the case of liposomes prepared with the thin layer hydration method during release studies.

The preparation of rutin loaded liposomes was carried out with the solvent injection and microfluidic method as well. With the optimization of the experimental conditions and purification method, ~75 and ~170 nm liposomes were formed with relatively good encapsulation efficiency values (~46% for both preparation methods). In addition to the presentation of the above-mentioned experimental results, the drug release studies will also be demonstrated.

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Acknowledgement: L. S. thanks the support of scholarship of University Researcher Scholarship Program (EKÖP-24-3-SZTE-578) funded by the Ministry of Culture and Innovation.

Ultrasonic fracture and dispersion of regular and novel carbon nanostructures: from graphite to soft mesoporous graphene frameworks

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ABSTRACT

Stable dispersions of carbon materials are becoming key precursors for composite carbon electrodes in energy storage and harvesting applications such as batteries, supercapacitors, and solar cells. One powerful approach to formulate these is ultrasonic irradiation. Our research covers the investigation of the ultrasound-assisted degradation of four carbon materials of distinctive structure and physicochemical properties [1]. Three of the most basic carbon material structures (graphite (Gr), carbon nanotube (CNT) and activated carbon (AC)) were investigated and compared to a novel graphene derivative: mesoporous soft 3D graphene framework, or graphene mesosponge (GMS), as schematized in Figure 1. The effect of mechanical input on the structural collapse and particle fragmentation is characterized by an extensive set of instrumental analysis. This first systematic study not only explored dispersion characteristics but also managed to correlate the mechanical degradation of basic classes of conductive carbon materials with their dimensionality and material properties such as bulk modulus.

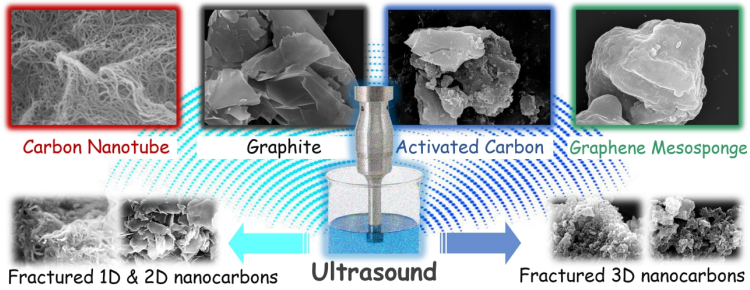

Figure 1. Generalized scheme of the research relying on ultrasonic fracture of 4 types of carbon materials.

The authors thank the support of the NKFIH (project No. 2019-2.1.7-ERA-NET-2021-00029) in the frame of supporting the AtomDec Consortium by the Visegrad Group-Japan 2021 Joint Call on Advanced Materials.

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The Effect of Surfactants on Polyelectrolyte Multilayer Nanofiltration Membranes

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ABSTRACT

The Layer-by-Layer (LbL) assembly technique for constructing nanofiltration membranes on ultrafiltration and microfiltration substrates has become an established method of advanced membrane fabrication, enabling the development of highly selective and chemically robust membranes [1]. These membranes exhibit notable self-healing capabilities and exceptional chemical stability, including resistance to chlorine, broad pH tolerance, and solvent resilience—provided the underlying substrate supports such conditions.

Despite these advantages, a known limitation of LbL membranes is the vulnerability of polyelectrolyte multilayers to destabilization under extreme conditions, such as high salinity (above 2–3 mol/dm³) or the presence of surfactants exceeding their critical micellar concentration (CMC) [2]. The effects of sub-CMC surfactant concentrations, however, remain largely unexplored. Understanding these interactions holds practical significance beyond fundamental insights, particularly for applications involving complex feedwaters—such as industrial wastewater or food processing streams—where low levels of surfactants are frequently encountered.

In this study, we systematically investigate the impact of gradually increasing concentrations of both cationic and anionic surfactants on the performance of LbL membranes, assessing flux and solute rejection characteristics. Based on the observed changes, we propose a mechanistic hypothesis for the onset and progression of membrane degradation under sub-CMC surfactant exposure.

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ACKNOWLEDGEMENT

This work has been implemented by the TKP2021-NKTA-21 project with the support provided by the Ministry of Culture and Innovation of Hungary from the National Research, Development, and Innovation Fund, financed under the 2021 Thematic Excellence Programme funding scheme.

Computer Simulation Investigation of the Molecular Scale Structure and Dynamics of the Free Surface of Imidazolium-Based Ionic Liquids

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ABSTRACT

The structure and single-particle dynamics at the surface of four imidazolium-based room temperature ionic liquids have been investigated by means of molecular dynamics simulations combined with intrinsic surface analysis (ITIM) [1] at both the molecular and atomic levels, further supported by Voronoi analysis. This methodology enabled us to explore the interfacial properties of these systems in unprecedented detail. We find no indication of either a double-layer-like ionic arrangement or the so-called "chessboard" pattern of self-association at the liquid–vapour interface. Instead, our results show that alkyl side chains of the cations aggregate into apolar domains that extend into the vapour phase, while the charged components are located in more embedded interfacial regions. Although the outermost layer is dominated by cations when viewed at the level of whole ions, the surface carries a small but distinct negative charge. This apparent contradiction is explained by the spatial structure: the alkyl chains obscure the imidazolium rings, while the smaller and more mobile anions can approach the free surface more readily, giving rise to the observed net surface charge. This excess charge could only be identified by applying intrinsic analysis. Regarding the interfacial dynamics, we find that the motion of individual ions at the surface is slowed by two to three orders of magnitude compared to that in typical molecular liquids. Lateral diffusion is found to be a generally slower process than the exchange of the ions between the subsequent subsurface layers.

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Bimetallic nanoclusters: Synthesis optimization and biological studies

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ABSTRACT

Noble metal nanoclusters (NCs) are unique materials with features different from classical nanoparticles. They show tunable fluorescence which can be utilized in many fields like sensing, labeling and imaging. The emission properties can be modified by selecting their stabilizing ligands and metal composition. The utilization of proteins like serum albumins, gamma-globulin, lysozyme and transferrin facilitates their biocompatibility.

Our main task was to prepare bimetallic gold-silver NCs by using the selected proteins as stabilizing ligands. We used the abovementioned proteins in high pH conditions which promotes their reducing ability. By optimizing different aspects of the reaction such as gold:silver ratio, protein and total metal concentration, temperature and synthesis time we can finely tune their emission maxima and enhance their fluorescence. The NCs underwent a cleaning process and were characterized to reveal the changes in protein structure and metallic core. Specifically, circular dichroism and Fourier-transformed infrared spectroscopy revealed the disrupting effect of NC formation on protein secondary structure. Mass spectroscopy was used to check the metal concentration after cleaning and their oxidation state was determined by X-ray photoelectron spectroscopy. Nanocluster size and hydrodynamic diameter were measured with transmission electron microscopy and dynamic light scattering. Aside from the detailed characterization, biological studies are also included in this presentation. To check the biocompatibility of the NCs, different cytotoxicity tests were run. Cell viability studies were run on several human cell lines, which ensures the NCs' applicability in medical and biological fields. In addition, based on their silver content, antibacterial characteristics were also tested on different Gram-positive and Gram-negative bacteria.

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ACKNOWLEDGEMENT

Á. Turcsányi thanks the support of scholarship of University Researcher Scholarship Program (EKÖP-24-3-SZTE-597) funded by the Ministry of Culture and Innovation.

Nanofibrous dual polymer meshes for surgical tissue regeneration

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ABSTRACT

The next generation of tissue engineering solutions is focused on designing multifunctional composite materials capable of simultaneously addressing multiple clinical challenges. A persistent challenge is achieving effective tissue integration of surgically implanted scaffolds. In this study, we present the development of advanced electrospun composite meshes composed of poly(succinimide) (PSI) and polycaprolactone (PCL), engineered to enhance tissue integration while maintaining robust mechanical properties. PSI, a synthetic poly(amino acid) known for its versatile chemical reactivity, offers extensive functionalization potential, whereas PCL is a widely used biodegradable polymer distinguished by its excellent mechanical strength and controlled degradation profile. While PCL exhibits a slow degradation rate (6 months to 2 years), which can hinder rapid tissue incorporation, PSI rapidly degrades unless stabilized through chemical cross-linking. We fabricated two distinct nanofibrous mesh configurations via electrospinning: (a) co-electrospun PSI/PCL meshes and (b) blend electrospun PSI/PCL meshes. Comprehensive characterization was performed, encompassing physicochemical, mechanical, and wettability assessments. *In vitro* cytocompatibility was evaluated using fibroblast cell lines, and *in vivo* biocompatibility was assessed in a Wistar rat model. The composite PSI/PCL meshes demonstrated superior mechanical performance, achieving nearly double the tensile strength of PSI-only meshes. The incorporation of PSI significantly enhanced hydrophilicity, as indicated by reduced water contact angles, thereby promoting favorable cell adhesion. Both mesh types exhibited excellent cytocompatibility and biocompatibility, supporting cell proliferation without signs of adverse tissue reactions. This work highlights the synergistic potential of PSI/PCL composite meshes, combining the mechanical durability of PCL with the versatile functionalization and rapid degradation of PSI. Such a composite approach not only addresses the inherent limitations of individual polymers but also provides a versatile platform for diverse biomedical applications, ranging from wound healing to tissue engineering scaffolds.

Thermal transport and coupling effects in molecular liquids and aqueous solutions under thermal gradients

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ABSTRACT

Thermal gradients can profoundly influence the physicochemical properties of liquids by inducing complex coupling phenomena between heat, mass, and electrostatic fields. In this work, we discuss recent advances in understanding thermal transport and polarization effects in aqueous electrolyte solutions and molecular liquids such as water and ethanol [1-3]. Thermal polarization refers to the electric field induced by molecular orientation in polar fluids when they are exposed to a temperature gradient [4]. Employing non-equilibrium molecular dynamics simulations with the TIP4P/2005 water model, we demonstrate that supercooled water features minima in thermal conductivity alongside an enhancement in thermal polarization [1]. This behavior is connected to the anomalous thermodynamic properties of water, including isobaric thermal expansion and isothermal compressibility, which emerge from the hypothesized second critical point. We have extended our investigation to ethanol, finding that it exhibits significant thermal polarization under temperature gradients, particularly when approaching its critical point [3]. This phenomenon mirrors that observed in water under near-critical conditions and can be explained using a theoretical equation that relates the thermally induced polarization to the isobaric thermal expansion [5]. The insights obtained from non-equilibrium simulations underscore the interplay of thermodynamic, structural, and dynamic properties at the molecular level, providing routes for novel applications related to thermally driven processes in soft matter.

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Mechanical Behaviour of Fibrous Materials

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ABSTRACT

Fibrous materials are becoming critical technological applications due to their high mechanical performances and low mass. When the fibrous texture is subjected unidirectional strain along one of the axes, the deformations are inherently nonlinear and the corresponding stress depends on the underlying material properties and damage formation. Little is known on the deformation mechanism, as well as the load bearing capacity of these materials. Unidirectional strain-controlled experiments on artificial fibrous electrospun networks have been studied. The main aim was to classify the essential mechanical and structural parameters that control the elasticity of fibrous tissues. Experimental technique combined with the statistical theories provide significant potential for the characterization of fibre texture during deformation and suggests reliable mechanical models for the unusual elongation behaviour. In the low strain regime. the force has an approximate linear relationship. At higher elongation, the slope of this dependence is continuously decreasing and the stress reaches a maximum. Then, increasing the extension, the force declines. Detailed analysis of the shape of the loading curves were carried out by enlarging parts of the loading curves. We have found at small scale that the loading curves show tooth-like profile. These experiments reviled that the unusual loading curve is the result of continuous stiffness reduction caused by damage formation due to either rupture of adhesive fiber-fiber bond fracture or degradation. The microscopic failure processes give rise to macroscopic deformation. Two basically different theoretical approaches have been introduced recently. The Fiber Bund Model (FBM) and the Sacrificial Bond and Hidden Length (SBHL) model. The FBM model takes into account the fibre breaking during deformation, the SBHL model describes the effect of fiber slipping and uncoiling. Both approaches result in similar sequential force drops during elongation, however the FBM model predicts stiffness reduction, while the SBHL model predicts toughening during elongation. Our assumption was based on that in real weak fibrous texture, both fiber sliding and unfolding as well as fiber splitting occur during deformation. An effort is made to interpret of the unusual mechanical properties of weak texture on the basis of FBM and SBHL models. Numerical simulations provide a better understanding of mechanism of deformation. The reported experimental and theoretical techniques have significant potentials for the characterization of fiber texture and suggests a further numerical simulations and development of probabilistic models for the load bearing behaviour of electrospun fibres.

Poster presentations

Freeze-dried liposomes for inhalation

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ABSTRACT

Inflammatory lung diseases such as asthma and COPD affect hundreds of millions of people worldwide. Inhaled products currently on the market are not liposomal, even though these nanoscale drug delivery systems have fewer side effects, can provide controlled drug release and better absorption due to their surfactant phospholipid shell. Our work aims to prepare liposomal drug formulations in powder form for inhalation and investigate their several parameters. The liposomes in the samples are around 100 nm in diameter and consist of a 3-component phospholipid bilayer and budesonide as an anti-inflammatory active ingredient. [1] The most important aspect of the studies is optimizing freeze-drying to increase shelf life. In particular, the optimal ratio and quality of disaccharide added to the samples for cryoprotectant purposes, as well as the concentration of the active ingredient, were determined. Dynamic light scattering measurements and scanning electron microscopy results indicate that a budesonide content of 10 m/m% is the most advantageous among the rehydrated samples for preserving the liposomal structure during freeze-drying. Both lactose and trehalose proved to be promising cryoprotectants in a phospholipid-disaccharide mass ratio of 1:15. Further investigations include the identification of possible interactions between different components by infrared spectroscopy, the acquisition of structural information using freeze-fracture electron microscopy, as well as the determination of the entry rate into the lower airways by means of a cascade impactor.

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Comparative analysis of virus nucleic acid extraction methods from wastewater samples

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ABSTRACT

Viruses are invisible pathogenic agents that can be injurious to humans, animals, plants, and even bacteria. The presence of viruses can be examined by detecting their genetic material. Several viruses can be found in communal wastewater. Utilizing an appropriate sample processing method is essential, as wastewater contains numerous inhibitory substances that can interfere with molecular analyses. This study compares two sample preparation methods – a traditional procedure (P) [1], [2] and a commercial nucleic acid isolation kit (K) [3] – that operates on similar principles. Wastewater samples from the wastewater treatment plant of Nagykanizsa were spiked with inactivated SARS-CoV-2 (novel coronavirus) control material (100 ul/L) to obtain detectable results. Virus-specific detection was performed using a Bio-Rad CFX Opus 96 real-time PCR thermocycler. None of the SARS-CoV-2 spiked samples (n=9), processed with the isolation kit, tested positive during the specific PCR. Inspite of three separate concentrations and triplicate sample processing. However, the same spiked wastewater gave a positive signal using the (P) method. Unidentified inhibitors and non-coronavirus-specific concentration steps can both be responsible for the lack of signal in the case of the enveloped RNA virus during (K) type concentration. Meanwhile, all the samples tested positive (both P and K methods) for adenovirus, a non-enveloped DNA virus. Significant differences between the two methods include initial sample volume, processing time, and incubation time; each factor can influence the outcome. In one hand, the commercial kit is user-friendly, quicker, and pre-packed, on the other hand, the non-commercial protocol can use a larger sample quantity, is freely modifiable, and is adaptable to research. The (P) protocol was considered more reliable for enveloped RNA viruses (e.g. SARS-CoV-2) than the (K) extraction kit.

ACKNOWLEDGEMENT

Financial support was received from the National Research, Development and Innovation Office (grant no. 2020-1.1.6-JÖVŐ-2021-00007).

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Characterization of immobilased enzyme kinetics on magnetic nanoparticles

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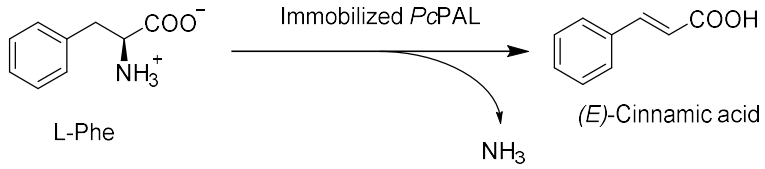
ABSTRACT

The aim of our research is to characterize the kinetic parameters of an enzyme immobilized on magnetic nanoparticles. As a model enzyme, we used recombinant phenylalanine ammonia-lyase from parsley fused to a polyhistidine affinity tag, which catalyses the ammonia elimination reaction of L-phenylalanine.



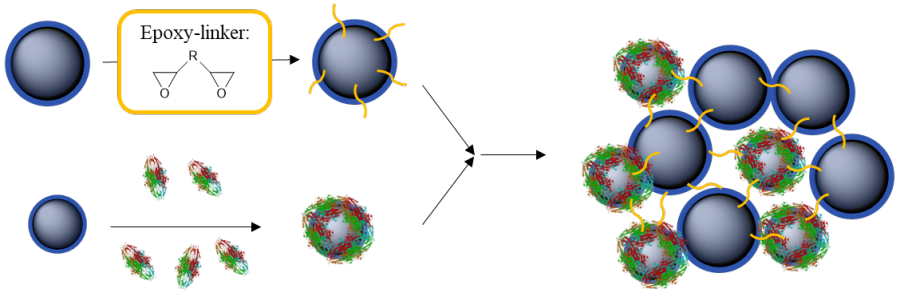
***1. Figure** The test reaction of* Petroselinum crispum *PAL*

The magnetic nanoparticles prepared by a solvothermal process were coated with aminosilane to form a surface containing amino groups. Various di- and triepoxy compounds were reacted on the amino groups and then the *Pc*PAL enzyme is attached to them.

The biocatalysts were determined according to the Michaelis-Menten enzyme kinetics parameters and the one showing the highest activity from the different epoxy compounds was selected from and used for further studies.

In addition, another biocatalyst was prepared by the magnetic nanoparticles containing surface amino groups were doped with EDTA complexing agent and complexed with cobalt ions, to which the enzyme was bonded via its affinity tag.

This final biocatalyst was cross-linked with MNP containing epoxy groups and the kinetic parameters and activity of the enzyme on the final cross-linked biocatalyst were investigated.



2. Figure The preparation of the cross-linked biocatalyst

Structuring liquids through solvent-assisted interfacial association of oppositely charged polyelectrolytes and amphiphiles

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ABSTRACT

The spontaneous formation of an interfacial membrane[1] at the water–undecanol interface, resulting from the association of an anionic polyelectrolyte (sodium polystyrene sulfonate, NaPSS) and a cationic single-chain surfactant (hexadecylamine, HDA), requires the incorporation of a long-chain alcohol as a co-surfactant. This phenomenon was confirmed through detailed analysis of the resulting solidified interfacial layer. The interactions between the polyelectrolyte and the surfactant were investigated at the toluene–water interface. Although interfacial precipitation was observed under these conditions, a continuous membrane did not form, and the two liquid phases could not be structured in a well-defined manner. Attenuated total reflection infrared (ATR-IR) spectroscopy measurements indicated that toluene is not incorporated into the precipitate. In contrast, the incorporation of undecanol is essential for the formation of a cohesive, solidifying interfacial layer, enabled by the surface freezing behavior of undecanol. Therefore, the resulting membrane exhibits temperature-responsive characteristics. Furthermore, it was also studied whether the layer is suitable for permanent stabilization of emulsion droplets. The interfacial film stabilizes emulsions containing toluene and undecanol as the organic phase in distinct ways, depending on the composition, further highlighting the role of undecanol in modulating membrane structure and interfacial properties.

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Role of Fluorocarbon Chain Length in the Adsorption of Perfluoroalkyl Substances on Nanoplastic Particles

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ABSTRACT

Emerging contaminants such as nanoplastics (NPLs) and per- and polyfluoroalkyl substances (PFASs) coexist in aquatic environments. Adsorption and aggregation processes were investigated in dispersions containing positively charged amidine-functionalized (AL) and negatively charged sulfate-functionalized (SL) polystyrene NPLs (approximately 100 nm) and PFBS (C4), PFHxS (C6) and PFOS (C8) in NaCl, $CaCl_2$ and $LaCl_3$ solutions. Electrophoretic light scattering and dynamic light scattering were applied to determine zeta potentials and hydrodynamic radii. Negatively charged PFASs adsorbed on oppositely charged AL, producing charge neutralization and charge reversal; the affinity followed the sequence C4 < C6 < C8. The particle dispersions aggregated rapidly at the isoelectric point, and the destabilizing PFAS concentration (DPC) correlated linearly with the isoelectric point in all electrolytes, confirming that electrostatic double-layer and van der Waals forces governed aggregation. Multivalent cations coadsorbed with PFASs, suppressed charge reversal and broadened the instability window. In SL systems, no significant interaction was observed, and colloidal particle stability was influenced by salt valence rather than PFAS dose. These observations provide quantitative information for predictive tools describing transport of PFASs by NPLs in aqueous samples of different ionic environments and highlight ionic composition, surface charge and fluoroalkyl chain length as key factors governing joint migration of NPL–PFAS adducts.

ACKNOWLEDGEMENTS

This research was supported by the National Research, Development and Innovation Office via Projects TKP2021-NVA-19 (jointly with the Ministry of Innovation and Technology of Hungary) and SNN142258.

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Role of fluorocarbon chain length in the adsorption of perfluoroalkyl substances on nanoplastic particles, ACS ES&T Water, 2024, 4, 5114–5121

Fabrication of poly (amino acid) based meshes for enhanced postoperative pain relief

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ABSTRACT

Introduction: Effective management of post-operative pain is a fundamental aspect of Enhanced Recovery After Surgery (ERAS). While NSAIDs are widely utilized for pain control, their use carries increased risks of nephrotoxicity and gastrointestinal complications. Similarly, opioids, despite being viable options, are associated with side effects such as respiratory depression, nausea, vomiting, constipation, and urinary retention. Local anesthetics (e.g. lidocaine, bupivacaine), on the other hand, has demonstrated potential in mitigating early post-surgical pain and promoting improved recovery. However, intramuscular administration of local anesthetics typically yields pain relief for only about 90 minutes. Incorporating local anesthetics within surgical meshes could prolong its therapeutic effect, thereby enhancing the post-surgical recovery process.

Objective: The aim of this study was to engineer a fibrous mesh with distinct chemical and physical characteristics, providing a novel strategy for post-operative pain management.

Materials and Methods: Polysuccinimide (PSI) was prepared through thermal polycondensation of L-aspartic acid according to an established method. The local anesthetic was mixed with the PSI, producing our working solution.The mesh was fabricated via electrospinning, followed by thorough evaluation of its chemical makeup, structural morphology, and mechanical properties. Analytical methods included ATR-FTIR spectroscopy, scanning electron microscopy, uniaxial mechanical testing, and UV-Vis spectroscopy.

Results: The successful fabrication of PSI meshes was validated using ATR-FTIR spectroscopy. Scanning electron microscopy indicated that the fibers had an average diameter of 450 nm ± 100 nm, confirming the appropriate structural formation. Mechanical testing demonstrated the mesh's suitability for implantation. The drug release studies showed that the majority of the local anesthetic was release within the first 5 minutes of the experiment, however minimal drug release continued for 5 hours.

Conclusion: The developed meshes display characteristics suitable for implantation, and preliminary data from UV-Vis spectroscopy on the drug release profile appear favorable. Next steps include in vitro cell studies and in vivo animal trials to further assess performance.

Monolayer-forming properties of bovine serum albumin and its composite multilayers on solid surfaces

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ABSTRACT

Thin films have a wide range of applications, e.g. in medicine or packaging. The protein thin films among these have big importance, because they can be multilayered into composite thin films with various substances (e.g. clay minerals). Such material could be graphite oxide, which is ideal for film building due to its lamellar structure.

The aim of this study was to investigate the formation and reproducibility of a bovine serum albumin monolayer and its multilayers built up with graphite oxide. The layers were constructed by layer-by-layer technique on pre-cleaned quartz plate substrate from an aqueous solution of albumin and an aqueous suspension of graphite oxide (Fig.1). The film formation was monitored by UV-visible spectroscopy and X-ray diffraction. The surface thickness and homogeneity of the films were examined by atomic force microscopy.

Experimental results showed that albumin monolayer forms very rapidly, in seconds, but its reproducible deposition is rather difficult, highlighting the importance of proper surface pre-treatment and steady ambient conditions. Multilayers are much easier to be reproduced, but their thickness is highly dependent on pH, because particle adsorption is greatly reduced with increasing alkalinity. Just as the protein on the quartz surface, graphite oxide forms fairly homogeneous layers on the protein-coated plate.

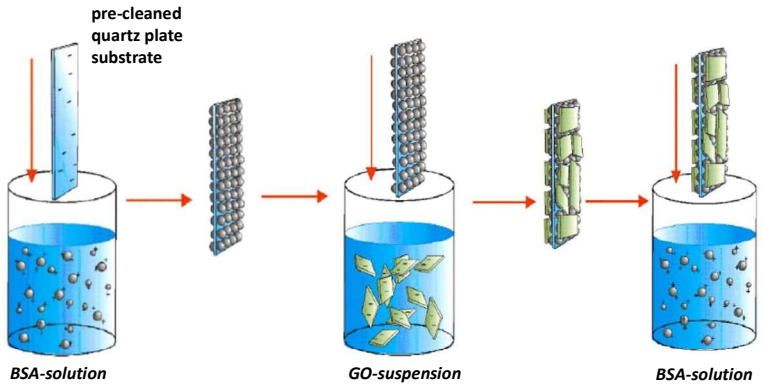

Figure 1. Generalized scheme of the thin layer deposition procedure of the protein/GO multilayers.

The authors thank the support of the NKFIH (project No. 2019-2.1.7-ERA-NET-2021-00029) in the frame of supporting the AtomDec Consortium by the Visegrad Group-Japan 2021 Joint Call on Advanced Materials.

Modeling Asymmetry in Flat Bilayers and Exosome-Like Vesicles: A Focus on Cholesterol Dynamics under Temperature Gradients

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ABSTRACT

In this work, we study cholesterol flip-flop under non-equilibrium conditions, focusing on the role of thermal gradients in promoting membrane asymmetry. We investigate this phenomenon in two systems: flat lipid bilayers and curved vesicle membranes resembling 30nm exosomes. Coarse-grained (CG-Martini3) Non-Equilibrium Molecular Dynamics (NEMD) simulations are employed to explore how temperature gradients influence cholesterol distribution and flip-flop dynamics in both systems.

In flat bilayers, we examine the behavior of cholesterol in different lipid membranes with each of the following phospholipid components, DLPC, POPC, DPPC and DLigPC. Each system contains a 50:50 cholesterol-to-phospholipid ratio, forming a liquid-ordered (Lo) phase. Under increasingly large temperature gradients, we observe enhanced cholesterol accumulation in the colder lipid leaflet, with an estimated Soret coefficient on the order of 10^{-3} K^{-1}, leading to increased membrane asymmetry. The study also explores the relationship between the length and saturation of the hydrocarbon chains of phospholipids, and their influence on cholesterol dynamics and the time constants to reach steady-state asymmetry.

We extended our analyses to vesicles to investigate the combined role of thermal gradients and curvature on cholesterol partitioning. In curved asymmetric vesicles with a 50:50 cholesterol-to-DPPC ratio, cholesterol preferentially accumulates in regions of negative mean curvature, leading to a redistribution towards the inner leaflet under thermal equilibrium conditions. We further examine the cholesterol distribution under temperature gradients and time constant for reaching the steady-state asymmetry.

This research provides valuable insights into the interplay between membrane curvature, cholesterol dynamics, and thermal gradients in vesicles and bilayers mimicking biological membranes. By advancing our understanding of cholesterol distribution and flip-flop dynamics, this study helps shed light on some of the mechanisms driving membrane asymmetry and controlling membrane stability.

Development and Characterization of Fiber-Reinforced Biodegradable Packaging Materials

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ABSTRACT

The medical sector enormously contributes to the waste disposal crisis. The problem is primarily caused by the packaging of medical devices intended for single use, for which biodegradable packaging materials made from bioplastics may provide an alternative. Polysuccinimide (PSI) is a potential base material for producing such fiber-reinforced biocomposite packaging.

Our aim was to create fiber-reinforced biocomposites and optimize the parameters involved, to examine the structural, mechanical, and thermal properties of the produced materials.

The fiber mats were produced by electrospinning from a solution of PSI. For the production of the composites, the mats were embedded in poly(lactic acid) (PLA) and poly(butylene succinate) (PBS) films by melting the matrix and impregnating the fiber with a hot-press. Structural analysis was conducted using scanning electron microscopy (SEM). The tensile strength and Young's modulus of the samples were measured using uniaxial tensile testing.

SEM images of the PLA/PSI composites showed that PLA completely impregnated the PSI fibers; however, due to low adhesion, the fibers easily separated from the matrix. In contrast, the PBS/PSI composites exhibited complete impregnation along with visible adhesion. The pressed PBS film showed a Young's modulus of 681±38 MPa and tensile strength of 31±8 MPa; for the PBS/PSI composite, the values were 663±24 MPa and 24±3 MPa. PBS/PSI composite with higher fiber load exhibited mechanical reinforcement compared to the initial composite samples. The sample's Young modulus was 1033±51 MPa and its tensile strength was 41±7 MPa.

These changes make the PSI/PBS based fiber reenforced composite a viable option in the development of new biodegradable composite materials.

Multi-Scale Mechanics of Cryopreserved Human Arterial Allografts Across a Six-Month Period

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ABSTRACT

Operating under septic conditions poses significant challenges in vascular surgery. Infection is a serious risk when handling synthetic vessel prostheses and is one of the most dreaded complications. In the event of graft infection, an infection-resistant alternative is necessary. Cryopreserved vascular allografts offer a suitable alternative to replace an infected vessel or a section of a synthetic graft. However, there are no international guidelines for the preparation, storage, and thawing of such vessel grafts.

Here, we aimed to investigate the mechanical properties of human cryopreserved arteries across multiple scales, ranging from nanonewton to newton forces and identify the optimal cryogenic storage duration.

Human arterial allograft samples were frozen in a slow, controlled process and stored at −80 ˚C. One native and four cryopreserved samples were examined during a six-month-long period. Dimethyl-sulphoxide was used as a cryoprotectant. The mechanical properties of fresh and stored samples were explored in uniaxial ring tests and nanoindentation.

We found no significant changes in the multi-scale mechanical properties during the examination period. Our results indicate that the cryopreserved vascular allografts are mechanically stable for up to six months under cryogenic conditions; hence, they represent ideal samples in vascular surgery. [1]

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AKNOWLEDGEMENTS

This research was funded by a grant from the Hungarian National Research, Development and Innovation Office (150826 to M.K.); NKFIH FK 137749 and TKP2021-EGA-23.

Fluidic Synthesis of Cationic Carbon Quantum Dots: Investigating Reaction Mechanism and Fluorescence Properties

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ABSTRACT

Carbon nanoparticles (CNPs) have emerged as promising alternatives to conventional nanomaterials, thanks to their strong photoluminescence, low toxicity, and adaptable surface chemistry. Nonetheless, traditional batch synthesis methods often suffer from low quantum yields and inconsistent particle sizes, while flow-based approaches, despite offering better control, face challenges such as handling high temperatures and managing gas evolution.

This study presents a rapid, reproducible method for synthesizing fluorescent CNPs via the alkaline hydrolysis of hexadecylpyridinium bromide (HPyBr) under batch conditions, with the aim of enabling a transition toward fluidic synthesis. The effects of temperature and reaction time on the structural, interfacial, and optical properties of the CNPs were systematically examined. The nanoparticles displayed strong hydrophobicity and a narrow size distribution ranging from 3 to 5 nm, with particle size increasing as reaction time lengthened. Additionally, they exhibited positive *ζ*-potentials, which progressively declined from +37 mV to +20 mV with longer reaction durations. Optical analysis showed broad UV-Vis absorption and stable blue–green fluorescence in organic solvents, with consistently similar spectral profiles observed across all samples.

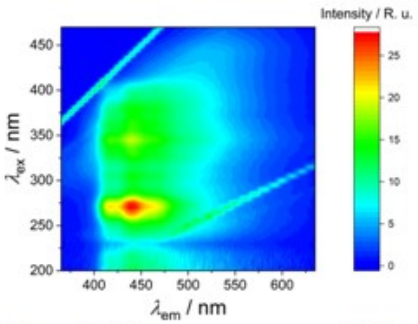

Figure 1. 3D fluorescence spectra of CNPs

Attenuated Total Reflection Infrared (ATR-IR) and Nuclear Magnetic Resonance (NMR) spectroscopic analyses suggest a micelle-templated ring-opening polymerization mechanism involving alkoxy-terminated imine intermediates and aldol-type condensation. Variations in particle size and *ζ*-potential among the samples were attributed to differences in the amount of precursor incorporated into the CNPs.

Based on these insights, a continuous fluidic synthesis protocol was developed and optimized. Nanoparticles produced in flow systems exhibited optical and structural characteristics similar to those synthesized in batch, with surface polarities varying according to synthesis parameters, as indicated by dodecane–water interfacial tension measurements.

These findings not only demonstrate the viability of fluidic CNP synthesis, but also provide into the nanoparticle formation mechanism. This work supports future efforts to tailor CNP properties for applications in sensing, imaging, and optoelectronics through scalable and tunable synthesis techniques.

Magnetite-reduced graphene oxide nanocomposite for the simultaneous removal of bisphenol A and glyphosate from aqueous solutions

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ABSTRACT

Rapid population growth coupled with intensified industrial and agricultural activities has led to widespread water pollution with contaminants of emerging concern (CECs). These pollutants pose substantial threats to all living organisms, compromise drinking water quality, and inflict environmental damage even at low concentrations. Among CECs, there are hydrophobic and hydrophilic compounds such as bisphenol A (BPA) and glyphosate (GLY), respectively. Both are endocrine-disrupting chemicals implicated in inducing mutagenic, carcinogenic, genotoxic, and neurological pathologies in human and animal populations. To mitigate these critical challenges, the current study successfully fabricated Fe_3O_4-rGO nanocomposite adsorbent via the solvothermal method [1] and applied it for the simultaneous removal of BPA and glyphosate from aqueous solutions. The TEM images confirmed the uniform dispersion of flower-like Fe_3O_4 structure on GO sheets, leaving enough space for the adsorbed hydrophobic molecules such as BPA, as well as iron oxide surface sites for GLY binding [2]. The zeta potential measurements further revealed a charge of -41.2 mV for the GO, signifying its surface is negatively charged and has exceptional colloidal stability in suspension. The adsorption experiments were quantified using UPLC-MS/MS, and the study was conducted under optimized conditions of 5.0 mg adsorbent dosage, 10 mmol/L N

aCl as an indifferent electrolyte, 55 rpm stirring, and a 24-hour reaction duration at room temperature. The results demonstrated remarkable removal efficiencies and adsorption capacities of 96.039% and 34.4 mg/g for GLY (at 100 mg/L initial GLY concentration), and 97.206% and 0.406 mg/g for BPA (at 1 mg/L initial BPA concentration), respectively. Generally, Fe_3O_4-rGO adsorbent emerges as a highly promising alternative for the simultaneous and efficient removal of hydrophobic and hydrophilic pollutants from water.

ACKNOWLEDGEMENT

This research was supported by the National Multidisciplinary Laboratory for Climate Change (grant number RRF-2.3.1-21-2022-00014).

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Fabrication and Mechanical Characterization of Polymer Fiber Systems in Physiologically Relevant Environment

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ABSTRACT

In reconstructive surgery, artificial implants and donor tissue are not always accepted by the patient's body. Nano- and micro-fibrous polymers have a structure that closely resembles the extracellular matrix (ECM) found in the living body, making them an ideal basis for artificial tissue supports. Poly(amino acids) are promising because they are easily degradable and do not trigger an immune response. The development of such fibrous materials, with their favorable mechanical properties, could open up new opportunities in a wide range of medical applications.

This research aims at the design and mechanical testing of an optimal ECM-like system that could be suitable for future medical applications.

Nanofibrous networks were created from polysuccinimide (PSI), the anhydride of poly(aspartic acid), by electrospinning. The mechanical behavior was studied during uniaxial and cyclic tensile tests. For the dry specimens, the effect of fiber orientation and tensile speed on the load carrying capacity were examined. For the tests in physiological environments, 1,4-diaminobutane (DAB) was used to cross-link the polymer chains, then uniaxial and cyclic tensile tests were performed to investigate the mechanical response.

I found that tensile speed has a small, while orientation has a significant effect on the mechanical properties of dry networks. The cross-linked specimens showed much higher elongation and elasticity, while they ruptured at significantly lower force levels, which were no longer affected by tensile speed. In the cyclic measurements, the dry meshes exhibited significant residual deformation and energy dissipation, while the cross-linked specimens were mechanically more stable. As the cycles progressed, the higher tensile speed increased the amount of deformation, but the absorbed energy and percentage of deformation remained at similar levels, indicating good load bearing capacity of the specimen.

In comparison with studies on porcine peritoneum, the mechanical response of cross-linked meshes showed a similar trend, bringing these synthetic systems closer to ECM-like behavior and potentially suitable for biomedical applications.

AKNOWLEDGEMENTS

We thank the NKFIH FK 137749 and TKP2021-EGA-23 for funding our research.

Biocompatible composite protective thin layer using sol-gel chemistry

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ABSTRACT

This study explores the synthesis and characterization of composite materials, focusing on the integration of silica cryogel and cellulose. The aim is to develop environmentally friendly, biodegradable thermal insulation thin continuous layers with optimized physical properties, like thermal conductivity adhesion on diverse surfaces, connection between the components of the composite. The continuous matrix phase of the composite is composed of cellulose fibers, known for their high thermal insulation capabilities, biodegradability, and abundant availability. Silica cryogel, selected for its excellent resistance to heat and chemical impacts, serves as the reinforcing phase. To improve the matrix-reinforcement phase connection, different additives were utilized, including a solvent mixture of NaOH and carbamide, and hydroxyethyl cellulose (HEC).

Characterization of the composite materials involved advanced techniques. Scanning electron microscopy (SEM) provided insights into the structure, morphology, and homogeneity, revealing the average pore size and overall porosity. Infrared spectroscopy (FT-IR) was used to identify bond structures and interactions between the composite components, providing a detailed understanding of the material's chemical composition.

The study puts a focus on the physical and chemical properties that arise from the interaction of silica cryogel and cellulose. The results demonstrate that the synthesized composites exhibit excellent thermal insulation and mechanical properties, highlighting their potential application in various industrial fields where thermal management and environmental sustainability are essential.

The final products were also subjected to thermal conductivity measurements, confirming their efficiency as insulating materials. The measured heat conductivity of 0.042 W/mK value of our composite is comparable to that of the commonly used mineral wool (Rockwool‘s product).

Adhesional measurements revealed strong bonding to diverse substrates, including metal, ceramic and glass, demonstrating the composite's practical applicability in various settings.

The integration of natural cellulose with synthetic silica cryogel represents a significant advancement in the development of sustainable materials, offering a promising solution for reducing the environmental footprint of thermal insulation products.

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Polycarboxylate coated Ni ferrite nanomagnets and the bio nano interface

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ABSTRACT

Magnetic iron oxide nanoparticles (MNPs) are well known for their great potential for biomedical use (e.g. drug-delivery, MRI contrast enhancement and magnetic hyperthermia). Beside magnetite, nickel-ferrite nanoparticles also seem to have promising magnetic properties for utilization in magnetic hypertermia. However, they require biocompatibilization with the application of a highly hydrophilic coating.

Nickel ferrite particles were prepared with a Ni content of 0%, 10% and 20%, and two different polycarboxylate type polymers (PAM and PEGMA) were used to fully coat the nanomagnets. The bare nanomagnets showed superparamagnetic feature and spherical morphology, and the mean diameter slightly decreased with increasing Ni content. All nanomagnets exhibited amphoteric surface charge characteristics, the IEP was varied between pH~6 and ~8 depending on the composition. Peripheral blood smears revealed excellent hemocompatibility for the studied NPs, while no thrombocyte aggregation and no change of the other blood constituents in the presence of the coated nanomagnets were observed. The interaction of the carboxylated ferrite NPs with plasma proteins showed notable differences depending on the coating procedure. We observed significant changes in the behavior of NPs, when the excess polymer was completely removed from the liquid phase (compaction). The compacted PEGMA coated NPs exhibited strong ‘shielding’ effect due to their superhydrophylic nature, while we obtained a subtle masking effect for the compacted PAM shells. Exposing the nanomagnets to an AC magnetic field for 5 minutes resulted in higher heat production with increasing Ni content.

ACKNOWLEDGEMENT

This research was supported by the Hungarian National Research Development and Innovation Office (NRDIH) through the FK131739 project and by the János Bolyai Research Scholarship of the Hungarian Academy of Sciences.

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Development of hydrophobically modified chitosan-pluronic nanoparticles for sustained and targeted drug release in ischemic brain tissues

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ABSTRACT

Although the human brain makes up only 2% of body weight, its energy demands are high, requiring at least 15% of the heart's blood output. When blood flow is impaired, brain ischemia occurs. In such a condition, anaerobic glycolysis occurs due to oxygen depletion, causing the pH to typically drop to 6.5–6.0. This ischemia with the associated chronic acidosis is one of the primary causes of brain damage and death. Drugs such as nimodipine (NIMO) and HC-067047 (HC) help treat ischemia but suffer from low bioavailability and lack of selectivity [1]. Thus, designing drug delivery systems to enhance solubility and selectivity is crucial. Chitosan nanoparticles (Chit NPs) can incorporate water-insoluble drugs, reducing toxicity while improving stability. Chit's reactive amino groups allow functionalization for optimized drug delivery. Reacting Chit with hydrophobic aldehydes yields compounds with varying pH-dependent solubility [1]. This can enable pH-induced drug release, which is essential for brain ischemia treatment. However, the focus now is not only on targeted release but also on prolonged drug delivery. Pluronic® F-127 (PF), a widely used biocompatible copolymer, helps achieve this [1]. We hypothesize that combining hydrophobically modified Chit polymer with PF can create multifunctional nanocarriers for targeted, sustained drug release in ischemic brain tissues (pH 6.5–6.0). These carbohydrate polymer-based nanocarriers could also enhance drug stability in aqueous mediums, making administration more effective.

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The authors thank the financial support from the Hungarian Scientific Research Fund (OTKA) K 134334 and PD 142293 (Á.D.). The authors thank the János Bolyai Research Scholarship of the Hungarian Academy of Sciences and for the financial support from the Interdisciplinary Research Development and Innovation, Center of Excellence, University of Szeged. K.W.K.A. is funded by a scholarship from the Hungary-Egypt joint executive program. This work also supported by the German Research Foundation (DFG), Research Unit RU2795: "Synapses under stress" (CRR: Ro2327/13-2, EF) and the EU's Horizon 2020 research and innovation program No. 739593.

Shear-induced catastrophic phase inversion of high oil content O/W emulsions

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ABSTRACT

High oil content oil-in-water (O/W) emulsions containing 70 % oil phase were prepared using sucrose esters or sorbitan esters as emulsifiers. Unlike the emulsion prepared with sorbitan esters, the sucrose ester-based emulsion exhibited higher viscosity and featured polyhedral oil droplets dispersed within a continuous water-phase network as observed by confocal laser scanning microscopy [1]. When shear force was applied, the network structure collapsed, resulting in catastrophic phase inversion, in which the dispersed oil phase transformed into the continuous outer phase [2]. This inversion was accompanied by a sharp decrease in viscosity and a noticeable increase in surface gloss due to exposure of the oil phase. Emulsion composed of sucrose esters exhibited superior UV protection and cleansing efficacy compared to that formulated with sorbitan esters. These enhanced functional properties are attributed to the shear-induced phase inversion, which allows the oil phase to act more effectively when it changes from a dispersed state to a continuous phase.

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ACKNOWLEDGEMENTS

This research was supported by Bio-industry Technology Development Project(No.20018375) funded by the Ministry of Trade, Industry and Energy

CPBCI 2025
15-19 June 2025
Eger, Hungary

Coarse-grained simulations of peptide *LGE*$1_{1\text{-}80}$

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ABSTRACT

Biomolecular condensates, such as P-bodies, nucleoli, and stress granules, play a crucial role in cellular regulation, including transcription, RNA metabolism, and ribosome biogenesis. Understanding their formation and organization is essential for uncovering the molecular basis of diseases like neurodegenerative disorders, cancer, and diabetes [1]. However, due to their structural heterogeneity and fast dynamics, capturing their organization requires a coarse-grained (CG) modeling approach that bridges atomistic details with mesoscale properties.

In this work, we develop a coarse-grained model based on atomistic potentials to study the formation of condensates of LGE$1_{1\text{-}80}$, a protein of interest in biomolecular phase separation and shown in Fig.1. Our approach aims at a **patchy model**, where interactions are coarse-grained in a way that preserves essential binding patterns while reducing computational complexity. We employ **cluster analysis** as a criterion to derive effective interactions, ensuring that the CG model retains key features of the self-assembly and phase separation observed in atomistic simulations.

By leveraging CG modeling, we extend simulations to longer timescales and larger system sizes, enabling us to explore whether biomolecular condensates form through **phase separation, self-assembly, or aggregation**. Our approach provides insights into the structural transitions of LGE$1_{1\text{-}80}$ within condensates and the fundamental mechanisms governing these transitions. This work contributes to the development of predictive models for biomolecular organization in crowded cellular environments.

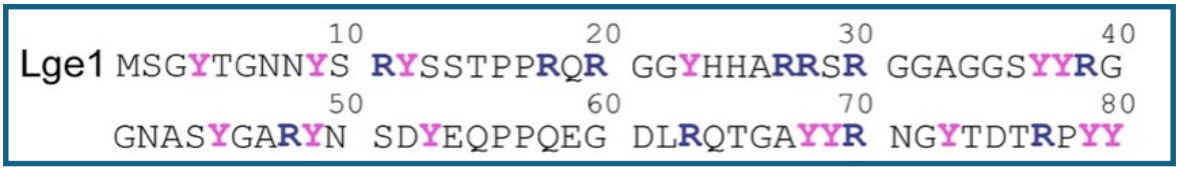

Figure 1. LGE1 1-80 protein used for coarse-graining.

Keywords: self-assembly, coarse-graining, phase separation

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Development of coaxial electrospun PSI fibers containing zinc and strontium salts for wound dressing application

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ABSTRACT

Currently, antibiotic resistant bacteria are becoming more common, necessitating the research for new solutions in wound treatment, such as the application of local antibacterial wound dressings. In my research, I prepared polysuccinimide (PSI) scaffolds using electrospinning in classical and coaxial configurations. The advantage of the coaxial structure lies in the prolonged release of active agents when the substance is located in the core of the fiber's core–shell structure. PSI is a biodegradable biopolymer suitable for use as a wound dressing material. Combined with zinc and strontium ions, it exhibits antibacterial and tissue-regenerating effects. I synthesized PSI and prepared polymer solutions containing salts (strontium nitrate, zinc acetate, and their combination), as well as salt-free variants. I measured the conductivity and viscosity of these solutions. The mechanical properties of the scaffolds were evaluated through tensile testing, their morphology was analyzed by scanning electron microscopy (SEM), and the presence of salts within the scaffolds was verified using energy-dispersive X-ray spectroscopy (EDS). Antibacterial activity was tested against four bacterial strains relevant to wound infections (*B. subtilis, E. coli, P. aeruginosa, S. epidermidis*). As a result, I found that viscosity and conductivity increased with salt concentration: 4.27 μS/cm for the salt-free polymer solution, 17.29 μS/cm with zinc acetate, 1180 μS/cm with strontium nitrate, and 942.78 μS/cm for the salt mixture. The increased conductivity was attributed to the presence of free ions, although the interaction between zinc and strontium ions reduced ionic mobility in the mixed solution. Salt content decreased mechanical properties (classical PSI: 0.36 Nm²/g; salt-containing samples: 0.09–0.14 Nm²/g), while the coaxial salt-free scaffold showed improved mechanical performance (0.46 Nm²/g). According to SEM analysis, fiber diameters ranged from 277 to 674 nm. EDS confirmed the presence of salts within the coaxial fibers. In the antibacterial tests, the salt-containing scaffolds produced inhibition zones around the scaffolds.

Acknowledgements:
This research was supported by NKFIH FK 137749 and TKP2021-EGA-23 research grants.

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Poly(aspartic acid) hydrogels with Priamine™ 1075 as a crosslinker

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ABSTRACT

Polymer hydrogels are very similar to human tissues, due to their large water content, porous structure and soft consistency; which make them particularly interesting for biomedical related developments, including drug delivery, tissue engineering, regenerative medicine or diagnostics. The tissue-like structure of hydrogels not just ensures a huge capacity for the entrapment of bioactive molecules that they are able to protect in hostile environment (e.g. the presence of enzymes and low pH in the stomach), but also promotes their biocompatibility. Responsive hydrogels have even more potential, as their volume (hence diffusion inside them and their optical properties) can be changed upon demand and consequently these hydrogels are able to control the release of their payload [1]. With the aid of such smart delivery systems drugs can be administered in a way that matches the physiological needs at the proper site and at the proper time, thus the shortcomings of the conventional drug formulations (such as burst release or poor bioavailability) could be overcome.

Poly(aspartic acid) (PASP), a synthetic poly(amino acid) is a well-known representative of biocompatible and biodegradable, pH-responsive, crosslinkable material, thus it can combine the benefits of synthetic and natural polymers. Crosslinking of PSI with a multifunctional primer amine in PSI leads to the formation of PSI gel, which can be easily hydrolized into PASP hydrogel.

In this work I aim to synthesize pH-responsive poly(aspartic acid) hydrogels by crosslinking polysuccinimide with a primer amine crosslinker, called Priamine™ 1075. Priamine™ 1075 dimer diamine is an ISCC PLUS certified product with 100% renewable carbon content (as opposed to the widely used crosslinker, 1,4-diaminobuthane [2], which is produced on an industrial scale by the hydrogenation of succinonitrile.)

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Binding characteristics of fluorescent probes to pillararene modified graphene oxide nanosheets and their implications for indicator displacement assays

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ABSTRACT

Fluorescent indicator displacement (FID) assays in which the macrocyclic host is grafted to a graphenic material have the advantage that they operate in *turn-on* mode, utilizing the FRET-type quenching of the graphenic component. As a contribution to the development of such sensors, we investigated the binding of a cationic and an anionic fluorescent probe, Oxazine 1 and Pyranine (HPTS) to a hybrid nanomaterial rGO-AP6 obtained by attaching a cationic pillar[6]arene (AP6) to reduced graphene oxide (rGO). The solid-state characteristics of this nanomaterial were unveiled using FT-IR, Raman and XP spectroscopy, while its properties in aqueous suspensions were investigated by UV-Vis, fluorescence and Zeta potential measurements. The binding of the two probes was investigated by adsorption studies at pH 6.4 and 10.2, using samples of low concentrations applicable in FID assays. It was found that rGO-AP6 binds HPTS strongly whereas the adsorption of OX is below the detection limit, which is opposite to the trend shown by the unmodified rGO adsorbent. The binding affinity of rGO-AP6 for HPTS could be tuned changing the pH. The AP6 units on the surface of rGO nanosheets proved to be closely homogenous binding sites for this anionic probe. These properties make the supramolecular system HPTS/rGO-AP6 a promising candidate as a fluorescent sensor for appropriate anionic biomolecules. In general, the findings of this study underscore the considerable potential of modified rGO nanosheets as platforms for FID sensors.

ACKNOWLEDGEMENT

[Financial support was obtained from the National Research, Development and Innovation (NRDI) Fund via research grant K143571. This work is a part of the projects BME-EGA-02 and NVA-04 supported by the Ministry of Culture and Innovation of Hungary from the NRDI Fund, under the TKP2021 funding scheme. E. K. gratefully acknowledges the support of the NRDI Office (research grant EKÖP-24-3-BME-175) and the research scholarship provided by ELTE Márton Áron Special College.

Microbial colonization and phenotypic resistance profile investigation across common polymer types

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ABSTRACT

Plastic pollution extends beyond its environmental footprint; microplastics are commonly found in wastewater and serve as artificial niches for microbial colonization and biofilm development [1]. These biofilms can include opportunistic pathogens and antibiotic-resistant bacteria [2], raising concerns for both ecosystem and public health. Six polymers: polystyrene (PS), polypropylene (PP), polyethylene terephthalate (PET), polylactic acid (PLA), polyvinyl chloride (PVC), and low-density polyethylene (LDPE) were selected based on their prevalence in aquatic pollution and consumer applications. Each polymer type was deployed in situ for environmental exposure, allowing biofilms to naturally form. After recovery, plastics were processed under sterile conditions. Cultivable microbes were isolated using selective agar media, including those targeting colistin- and carbapenem-resistant strains. Further phenotypic screening of antibiotic resistance profiles was conducted through standard growth assays, revealing patterns of susceptibility across a range of clinically relevant antimicrobials. A total of 314 bacterial isolates were obtained, with varying distribution across polymer types. The most frequently encountered genera included identified with MALDI TOF were: *Stenotrophomonas*, *Aeromonas*, *Morganella*, *Enterobacter*, and *Pseudomonas*. Diversity varied significantly among polymers: PS and LDPE supported broader microbial communities, while PLA and PET exhibited lower colonization. Material-dependent colonization trends were evident, including polymer-specific associations such as *Lactococcus lactis* on PP and *Yokenella regensburgei* on PVC. Resistance profiling revealed several strains capable of withstanding reserve and last-resort antibiotics, including colistin and carbapenems.

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New process for producing nanosilver

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ABSTRACT

The most important and well-known property of nanosilver is its antimicrobial effect, which makes it extremely effective in preventing and treating infections [1]. Nanosilver is also known to have antiviral effect, which can provide protection against certain viral diseases [2].

There are several methods for its production, the three main types being:

- chemical reduction methods [3],
- photoreduction methods [4],
- electrochemical methods [5].

In our experiment, nanosilver was produced by photochemical reduction, starting from a diammine silver(I)-solution, without adding any reducing agent.

Our method succeeded in producing high-quality nanosilver. The big advantage of our method is that it can be performed at home using commercially available tools and materials, with low environmental impact.

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Biopolymer-enhanced viscosity in salt solutions: effect of inorganic and organic cations

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ABSTRACT

The impact of inorganic salts and ionic liquids (ILs) on the solution properties of scleroglucan (SG), an increasingly used and researched fungal-origin biopolymer was investigated to broaden the range of potential applications [1].

In the present work, a combination of rheological, electrophoretic, and small-angle X-ray scattering measurements was performed in order to assess the viscoelastic, electrostatic properties, and structural properties in SG solutions.

The possible intermolecular interactions between the triple helical polymer chains were explored using rheology in both rotational and oscillatory modes under different experimental conditions. At moderate polymer concentrations, SG exhibits pseudoplastic flow behavior, and the presence of multivalent metal ions stabilizes the elastic character of these solutions even at high salt concentrations relevant to industrial applications.

Furthermore, high concentrations of monovalent salts disrupt the coherent structure of SG in solutions, as indicated by the striking increase in loss factor data. The coherency can be recovered by addition of imidazolium-based ILs (C_2-mimCl and C_4-mimCl) to the systems [2]. The ability to regenerate SG coherent structure with minimal IL concentrations provides an approach to reaching optimal rheological performance even at high salinity.

These findings emphasise the crucial role of chemical additives in tailoring the viscoelastic characteristics of SG solutions, demonstrating their potential in industrial applications requiring high-viscosity materials with well-defined viscoelastic behavior.

ACKNOWLEDGEMENT

The research project was supported by the National Research, Development and Innovation Office via project SNN142258.

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Enzyme Replacement Therapy via Silica-Immobilized Human Tyrosine Hydroxylase

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ABSTRACT

Human tyrosine hydroxylase (hTH) catalyzes the conversion of L-tyrosine to L-3,4-dihydroxyphenylalanine (L-DOPA), the rate-limiting step in dopamine biosynthesis. Dopamine is a critical neurotransmitter required for proper motor and cognitive function, and its deficiency is commonly associated with neurodegenerative diseases such as Parkinson's disease. Current treatments rely heavily on oral levodopa administration, which can lead to systemic side effects and diminished long-term efficacy.

As an alternative approach, enzyme replacement therapy (ERT) using recombinant hTH has the potential to restore local dopamine production. However, direct delivery of soluble enzymes poses challenges related to stability, aggregation, and bioavailability. To overcome these limitations, we investigated the use of silica nanoparticles (SNPs) as a platform for hTH immobilization. Recombinant hTH, fused with glutathione-S-transferase, was expressed in *E. coli* with high yield and purity. SNPs were synthesized with controlled particle sizes and surface-functionalized with amino groups to facilitate ionic binding of the enzyme. Immobilization consistently achieved >70% efficiency. Dynamic light scattering and zeta potential measurements confirmed improved colloidal stability and reduced aggregation after immobilization. Enzymatic activity of both native and immobilized hTH was confirmed via UV-Vis spectroscopy, monitoring the oxidation of L-DOPA to dopachrome.

These results highlight the potential of SNP-based hTH immobilization for ERT applications. The system offers enhanced enzyme stability and activity, with the added benefit of compatibility with intranasal delivery — a non-invasive route for targeting the central nervous system. Ongoing studies aim to optimize immobilization parameters and evaluate therapeutic efficacy in relevant in vitro penetration models.

Project NO.2024-2.1.2-EKÖP-KDP-2024-00005 has been implemented with the support provided by the Ministry of Culture and Innovation of Hungary from the National Research, Development and Innovation Fund, financed under the **EKÖP_KDP-24-1-BME-4** funding scheme.

Connections between the spread of respiratory diseases and the weather

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ABSTRACT

This study investigates the influence of weather conditions on the spread of respiratory diseases. Several scientific publications have addressed how specific pathogens responsible for respiratory infections respond to varying meteorological conditions [1].

While previous studies have examined the impact of different weather types on the transmission of such pathogens, our research further explores the role of topography—particularly whether valleys, due to their distinct mesoclimatic characteristics, influence disease transmission dynamics. Given that weather parameters can behave differently in valley regions compared to flat terrains under the same synoptic conditions, these variations may contribute to differences in infection rates. To assess this, we compare data from counties in Northern Hungary—characterized by a predominance of valley settlements—with counties in the Great Hungarian Plain. Our analysis utilizes data from the National Public Health and Pharmaceutical Center [2], the Hungarian Meteorological Service (Hungaromet) [3], and the FORESEE climate database maintained by the Department of Meteorology at Eötvös Loránd University [4]. The ultimate aim of this study is to develop a weather-type-independent model for predicting the spread of respiratory diseases.

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Preparation of Magnetite-containing Polymer Wound Dressing by Electrospinning

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ABSTRACT

Multidrug-resistant bacteria represent a significant challenge today, particularly in the treatment of chronic wounds. This problem is further complicated by the increasing resistance of these pathogens to conventional antimicrobial agents. Metal nanoparticles (MeNPs) offer a promising therapeutic alternative due to their ability to inhibit microbial growth through multiple mechanisms [1]. However, assessing their cytotoxicity is essential, as it is influenced by the physical and chemical properties of the nanoparticles [2], [3].

Our research aimed to develop a biocompatible, polymer-based wound dressing containing magnetite nanoparticles (MNPs), produced via electrospinning.

The biocompatible and biodegradable polysuccinimide (PSI) is a good candidate to create extracellular like structure from dimethyl formamide. Magnetite was synthetised through co-precipitation method then dispersed in the polymer solution. Although homogenizing MNPs in organic media proved challenging, we successfully created a stable dispersion. Dynamic light scattering (DLS) and UV-Vis spectroscopy were used to characterize the nanoparticles, while scanning electron microscopy (SEM) and FTIR was used for the fibre characterization. The antibacterial experiments were performed with 4 strains relevant for wound coverage (*E. coli, P. aeruginosa, B. Subtilis, S, epidermidis*).

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ACKNOWLEDGEMENTS

This research was supported by NKFIH FK 137749, TKP2021-EGA-23 research grants and the Semmelweis Travel Grant.

Colloidal (de)stabilization of graphene nanoplatelets using graphene oxide

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ABSTRACT

Due to its wide range of applicability, graphite oxide (GO) attract increasing research interest. However, GO bears inherent lack of good electrical conductivity. Another widely studied group of "graphene" materials is graphene nanoplatelet (GNP), which is significantly more conductive than GO due to its relatively extensive condensed aromatic ring system. At the same time, GNPs contain O-functional groups only at the edges of the nanoparticles, with a significantly lower quantity compared to GO, which seriously affect their aqueous dispersion stability. In this work, we explore the possibility to formulate composite dispersion of GO and GNP, in order to manage a reasonably good colloidal stability while maintaining excellent electrical conductivity of the graphene particles and their networks. As it is visually demonstrated in Figure 1, the dispersions of bare GNP and its composites with GO are markedly different under various solution conditions and GNP/GO ratios, and pH greatly affect the shelf-life of their dispersions.

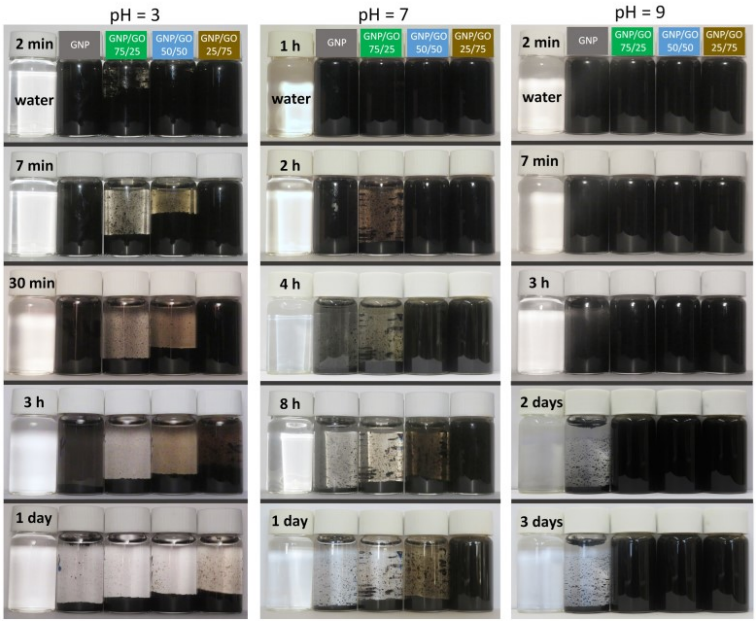

Figure 1 Photographs of undisturbed GNP/GO composite dispersions at different mass ratios and pHs.

The authors thank the support of the NKFIH (project No. 2019-2.1.7-ERA-NET-2021-00029) for the AtomDeC Consortium by the Visegrad Group-Japan 2021 Joint Call on Advanced Materials.

$CaCl_2$ transport in nanopores: competition of ions and water at the charged surface groups and the effect of charge scaling on selectivity

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ABSTRACT

Charge inversion in negatively charged nanopores is induced by overcharging the negatively charged surface groups by multivalent ions. This effect leads to a reversal of ionic selectivity in the nanopore. While the pore is a cation selective for 1:1 electrolyte, it is an anion selective for 3:1 electrolyte, with 2:1 electrolyte being in between. [1]

This work questions how to model the surface group to avoid non-ergodic behavior and reproduce experimental features. We expand the analysis of the control parameter q/d (charge-to-diameter ratio) to include confined geometries, building on our prior bulk studies. Trends in the RDF indicate specific behaviors of O- - Ca2+ interactions in proximity to pore surfaces. The RDF peaks for TIP4P/2005 exhibit a bulk-like sequence ECCR > ECCR2 > ECC, reflecting significant structuring of ions and water around the surface group O-, attributed to the balance of II and IW interactions. In contrast, SPC/E displays a reversed sequence ECCR < ECCR2 < ECC with modified peak intensities, indicating diminished hydration dynamics and a change in competitive adsorption between Ca2+ and water molecules. [2, 3]

The findings illustrate the dual competition wherein water molecules hydrate Ca2+ ions while simultaneously interacting with o- on the pore surface. TIP4P/2005 is identified as the most efficient model for accurately representing hydration effects in confined environments, whereas the reversed trend observed in SPC/E indicates its limitations in modeling these systems. This research highlights the significance of adjusting electronic charges and ionic diameters to obtain precise predictions of charge inversion phenomena and hydration dynamics within nanopores.

This research elucidates the impact of scaling parameters on charge inversion phenomena and transport characteristics within nanopores. The results indicate potential applications in the design of synthetic channels with customized selectivity and rectification characteristics.

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Engineered magnetic nanoparticles as advanced carrier materials for enzyme catalyst

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ABSTRACT

Enzymes are essential biocatalysts that enable a wide range of (bio)chemical transformations in living organisms and have become indispensable in numerous industrial sectors. Despite their high specificity and efficiency, the broader industrial implementation of enzymes is often limited by their low stability, high cost, and lack of reusability in homogeneous systems. To overcome these challenges, immobilization techniques have gained prominence, as they can significantly enhance enzyme stability, catalytic performance, and reusability. Among the various nanomaterials, magnetic nanoparticles (MNPs) are particularly attractive due to their large surface area, biocompatibility, and the ability to be easily separated from reaction mixtures using an external magnetic field[1]. In our research, we have focused on developing and optimizing enzyme immobilization strategies using magnetite (Fe_3O_4) nanoparticles as supports. We synthesized uniform Fe_3O_4 nanoparticles via a controlled co-precipitation method and tailored their surface properties through functionalization with various organosilanes, enabling covalent attachment of target enzymes. As model enzyme, lipase B from *Candida antarctica* was chosen for its industrial relevance and catalytic versatility. By optimizing the immobilization conditions -- such as organosilanes ratios and types and the used temperature -- we achieved high enzyme loading and retained a significant portion of catalytic activity after immobilization. The resulting biocatalyst exhibited improved operational stability and reusability and maintained high activity. Our findings demonstrate that careful design of the nanoparticle support and immobilization protocol can address key limitations of the enzyme usage in industrial applications, such as enzyme catalyzed polymer degradation. This work contributes to the broader adoption of enzyme-based technologies and highlights the potential of magnetic nanoparticle-supported immobilization systems for advancing industrial biocatalysis.

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Investigation of pH-dependent swelling of nanohydrogel fibrous fibers

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ABSTRACT

This presentation will discuss the morphology of poly(aspartic acid) gels crosslinked with 1,4-diaminobutane (PASPDAB) made by electrospinning and their pH induced swelling behavior. Due to the fact that these soft, fibrous hydrogel mats resemble the native tissue, there is an increasing interest in their research. However, the swelling properties of these hydrogel membranes is not yet fully understood. Therefore, we synthesized PASPDAB which shows pH-dependent swelling behavior and investigated its properties.

First, we synthesized polysuccinimide and confirmed its chemical structure by FTIR and measured its molecular weight using GPC-MALS (Mw 54.5 kg/mol, Đ 2.28). Then, fiber mats were synthesized using a custom-made electrospinning setup with a rotating drum collector. Fiber morphology was investigated by SEM and fibers typically had diameters in the range of 400-800 nm depending on the sample. Crosslinking was carried out by submerging the samples for 1h into 1,4-diaminobutane/ethanol solution. Then, samples were hydrolyzed in pH 8 buffer to form PASPDAB fiber mats. The chemical structure changes were confirmed by FTIR. SEM showed that the fibers in the fibrous samples slightly fused together during the crosslinking process, thus the mat transformed into an interconnected web. Samples were placed into pH 3 then pH 8 in repetitions to see the volume change, its kinetics and repetitiveness. The samples swelled in pH 8 and shrunk to about half of their size in pH 3. However, they did not show significant size change by submerging them in a broad concentration range of NaCl solutions. Based on kinetic observations, the total size change occurred in approximately 360 min and the change followed a sigmoidal curve in semi-logarithmic representation. Measurements showed that 50% of the size change occurred in 63 minutes during shrinkage and in 6 minutes during swelling.

These soft fibrous membranes are flexible and suturable alternatives for bulk gel implants which are many times brittle and fragile. It is our expectation that fibrous gels show much faster swelling response than their bulk counterparts.

Characterization of mucoadhesion of polymer tablets on a hydrogel surface applying tensile and shear stress

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ABSTRACT

By mucoadhesive dosage forms bioavailability of the drugs administered systematically or locally can be enhanced significantly [1]. Mucoadhesion tests generally use tensile load due to simplicity of the test, although shear is a more characteristic stress regarding mucosal tissues [2]. Here I developed rotational and oscillatory methods using a rheometer for testing mucoadhesion of solid polymer tablets and compared the results with those of conventional tensile tests. Due to the natural diversity, preparation and storing difficulties with natural tissues the *ex vivo* tests have poor reproducibility, thus a mucosa-mimetic material is needed and hydrogels can model the viscoelastic and adhesion properties of the mucosa and the mucus [3]. Poly(vinyl alcohol) (PVA) and mucin-containing PVA hydrogels, developed in our research group were used in this study as mucosa-mimetic materials [4]. Applying repeated shear load in rotational mode the reversibility of the adhesion was shown using hydroxypropyl methylcellulose (HPMC) tablets. Moreover, linear correlation between shear and tensile methods were shown using polyacrylic acid, HPMC and chitosan tablets.

Project no. EKÖP-24-2-BME-120 and project no. TKP-9-8/PALY-2021 have been implemented with the support provided by the Ministry of Culture and Innovation of Hungary from the National Research, Development and Innovation Fund, financed under the 2024-2.1.1-University Research Scholarship Program and TKP2021-EGA funding scheme. Further support was provided by the NRDI Office via grant FK 138029.

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Simulation-assisted Electrostatic Fibre Formation and Cellular Adhesion into the Nanofibre Structure

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ABSTRACT

Electrostatic fibre formation is a widely investigated and used non-mechanical technology that can be used to produce nano and microfibres. These fibre structures have wide applicability in medicine, pharmaceutical and in engineering. For medical purposes these structures are widely researched because they mimic the extracellular matrix thus making them an excellent candidate to be used in tissue engineering applications. [1] Outside of the applications in tissue engineering these fibre matrices are also excellent drug delivery systems because of the known dissolution rate therefore the dissolution rate of their delivered pharmacological substance. In medicinal applications they are also excellent candidates for antibacterial wound dressing where they deliver metal nanoparticles, antibiotics, or other antimicrobial materials. The nanofibre matrices also have applications outside of medicine, especially in filtration systems, new generational energy storage devices and in different biosensor systems.

The applications of the fibre structures are dependent on different physical and chemical properties; the chemical applications are dependent on the material conditions especially the solvent and the polymer that is used for the electrospinning. The physical properties are dependent on the machine and on the ambient parameters during the electrospinning. The focus of my presentation will be the mash modelling of the electric field during the electrospinning and the effect of the added CaCl2 on the created polymer fibre matrix.

The electric field modelling can give us a better understanding of the whole electrospinning process, especially of polymer deposition on the different collector geometries. These simulations can also lead to better collectors or needle geometries that can help to further optimize the polymer fibre formation.

The physical and chemical parameters of the fibre structure also depend on the chemical components of the electrospinning solution. During my research I investigated the effect of different CaCl2 concentrations in the Polysuccinimide polymer solution. The ionic salt content can affect the diameter of the fibre strands and can influence the cytotoxicity of the fibre structure.

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Wetting end evaporation on CNT- and ZnO-forests

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ABSTRACT

Recent developments in nanotechnology have highlighted the importance of the classical topics of wetting, spreading and evaporation due to their pronounced effect in technological applications. Arrays of vertically aligned 1D nanotubes and nanowires form so called forests structures, which offer unique characteristics not available with disordered states. The multifunctional carbon nanotubes (CNTs) are a typical candidate for the preparation of forest structures, but there are several other suitable materials, such as zinc oxide (ZnO). The main goal of this work was to obtain a more detailed picture of the surface properties (namely, wetting and vaporization) of the CNT- and ZnO-forests prepared by chemical vapor deposition (CVD) method and electrochemical deposition.

The vaporization of sessile droplets was studied first by contact angle measurements at room temperature after that by simultaneous weight monitoring and thermography at 50 °C [1-2]. There are several parameters characteristic for the evaporation process (initial contact angle, total evaporation time, time of evaporation only from the surface, evaporation rate, initial area of the droplet, *etc.*). It was proved by using statistical methods (*e.g.* Pearson correlation coefficients), that the experimentally determined values are specific for the physical properties of the solvents and for the quality of the solid materials. The results allow us to presume the possibility of this experimental setup and theoretical approach for a potential future application in the field of analytics.

ACKNOWLEDGEMENT

We acknowledge the support by the János Bolyai Research Scholarship of the Hungarian Academy of Sciences.

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Effects of electrolytes and polyelectrolytes on the colloidal stability and enzyme-like activity of CeO_2 nanozymes

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ABSTRACT

A network of enzymatic and molecular antioxidants is responsible for the decomposition of reactive oxygen species (ROS) in living organisms. Preventing the accumulation of ROS is crucial as high concentrations result in oxidative stress which is associated with several diseases including cancer, diabetes and cardiovascular conditions. Additionally, ROS can be responsible for the deterioration of the quality and storage stability of many industrial products. The use of natural antioxidant enzymes as highly efficient catalysts is limited by their costly and complicated extraction, transportation and storage alongside their sensitivity to environmental parameters. Enzyme-mimicking nanoparticles (nanozymes) provide a promising alternative due to their structural stability, inexpensive preparation and tunable physicochemical properties.

Maintaining the colloidal stability of nanozymes in the presence of various electrolytes at high concentrations is essential for their widespread application. Our work focused on the effect of monovalent salts on the dispersion stability and peroxidase-like activity of CeO_2 nanoparticles (CeNPs), a nanozyme known to mimic multiple native enzymes. Investigations were extended to both acidic and basic conditions as the colloidal properties of CeNPs are highly dependent on the pH of the dispersion. All tested combinations of cations (Na^+, K^+, Cs^+) and anions (Cl^-, NO_3^-, SCN^-) caused fast aggregation in low concentrations. A deviation from the Hofmeister series was observed as nitrate ions proved to be especially destabilizing. Nevertheless, the tested salts did not reduce the peroxidase-like activity of CeNPs even in high concentrations. The gathered data provides valuable information about a key parameter in most applications of CeNPs and underscores the need for further optimization of colloidal stability.

For this purpose, the surface of CeNPs was systematically functionalized with oppositely charged polyelectrolytes (PEs): heparin (HEP) and methyl glycol chitosan (MGC) were used at pH 4 and pH 10, respectively. The adsorption of PEs induced charge reversal of the dispersed particles and significantly improved their colloidal stability in salt solutions as demonstrated by the remarkable increases in critical coagulation concentration. Functionalization also resulted in substantially higher peroxidase-like activity highlighting polyelectrolyte-CeNPs systems as outstanding candidates for mimicking enzymes in high ionic strength environments.

Papain functionalized Prussian blue nanozyme colloids of triple enzymatic function

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ABSTRACT

In recent decades, it has been discovered that certain nanoparticles—so-called nanozymes—are capable of mimicking enzymatic activity. Unlike natural enzymes, however, they are not prone to several unfavorable properties, such as denaturation or high sensitivity to changes in pH, pressure, and temperature. Additionally, their production is significantly more cost-effective. One of the major challenges in this field is to develop a nanozyme system capable of multiple enzymatic functions simultaneously.

In our research, we functionalized Prussian Blue (PB) nanocubes with papain enzyme (PPN) and examined the resulting composite both from colloid chemical and biocatalytic perspectives. The physicochemical and morphological properties of the particles were characterized using dynamic and electrophoretic light scattering methods and transmission electron microscopy. The synthesis produced a nearly monodisperse aqueous dispersion with high colloid stability even at elevated ionic strength; aggregation could only be induced specifically with $MgCl_2$. The change in zeta potential and its signal reversal with increasing PPN dosage indicated that the effective binging of the enzyme to the PB surface. At the determined optimal 4:1 PB:PPN mass ratio approximately 90% of the PPN molecules were bound to the PB nanocube surfaces, as determined by the Bradford assay. The PB-PPN composite also demonstrated high stability even under high ionic strength conditions.

We confirmed that PB nanocubes exhibit superoxide dismutase- (SOD) and peroxidase-like (POD) enzymatic activity, which remained intact after papain immobilization. In summary, the nanozyme particles developed combines high colloidal and structural stability with being capable of both eliminating oxygen-containing free radicals and hydrolyzing proteins. These results may be of considerable interest, particularly in industrial processes where the application of natural enzymes is challenging.

ACKNOWLEDGMENT

The financial support of the National Research, Development and Innovation Office NANO-IBD 2024-1.2.3-HU-RIZONT-2024-00035) and the Hungarian Academy of Sciences (LP2022-16/2022) is acknowledged.

Interfacial thermal conductance of Janus nanoparticles

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ABSTRACT

Nanoparticles are of significant interest in medical, catalytic, and imaging applications. Gold nanoparticles, including gold nanospheres (1-100 nm in diameter) and gold nanorods (1-100 nm in length with a length-to-width ratio of 3-6), are popular due to their optical properties and ease of surface functionalization. These gold nanoparticles can also serve as nano-heaters in photothermal therapy applications. One major challenge in this area is adjusting their to target plasmonic wavelengths (800-1200 nm) that can effectively penetrate human tissue.[1] Another challenge is controlling the directionality of heat flow. Recently, we proposed an approach to achieve directionality using Janus nanoparticles (JNPs).[2] These JNPs incorporate various coatings that can control the heat flow direction. However, the interfacial thermal conductance (ITC) of JNPs is not well understood, complicating the nanoparticle design. Non-equilibrium molecular dynamics (NEMD) simulations provide a route to quantity the nanoscale heat transport and the interfacial thermal conductances.[3,4]

Here, we discuss NEMD simulations of cylindrical JNPs coated with hydrophilic ligands of varying carbon chain lengths and hydrophobic ligands of constant length. We computed their ITC with water. Heat transfer through the hydrophilic ligands is greater than that through the phobic ligands, leading to significant temperature variations at the nanoscale. Our study presents an approach to quantify the surface temperature of JNPs, providing insight into the design JNPs with adjustable heating properties.

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Development of selective sol-gel enzyme immobilization methods on magnetic nanoparticles

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ABSTRACT

The aim of the research is to develop a method for the rapid and selective immobilization of transaminase enzymes. It was implemented on a magnetic nanoparticle (MNP) functionalized with metal ion complexes responsible for selectivity. In the first step of the immobilization the histidine-tagged transaminase selectively forms a complex with the transition metal ion. Because of the selectivity purification of the target enzyme is not necessary the immobilization can be performed directly from the fermentation medium. After that, a sol-gel matrix was formed around the MNP and the immobilized enzyme for subsequent stabilization.

During the research several parameters were optimized. I examined the type of the aminosilane and also attached “inert” silanes to the surface of the nanoparticle mixed with the aminosilanes. In this way, the surface hydrophilic-hydrophobic properties of the particles can be influenced, and the number and distance of the binding sites can be controlled. All of these can affect the activity of the enzyme. During the sol-gel matrix formation the reaction time and the amount of the silane precursor were in the focus of the optimization process. Also the diffusion properties of network structure can be influenced by using mixtures of different silanes.

I performed the attachment process with the *Vibrio fluvialis* (*S*)-selective transaminase enzyme. I examined the prepared biocatalysts in the conversion of α-methylbenzylamine, from which the resulting acetophenone can be easily detected in UV. I also examined the activity of catalysts enclosed in a sol-gel matrix and without subsequent stabilization in the reaction.

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