Alpine NMR Workshop

Recent advances in NMR methods and applications to materials

Bled, September 18-22, 2025

Abstract book

Editors: Aleš Mohorič, Igor Serša

Faculty of mathematics and physics, University of Ljubljana

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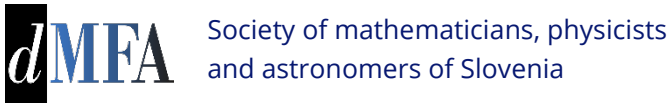
Society of mathematicians, physicists and astronomers of Slovenia



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FOREWORD

The Alpine NMR Workshop on *Recent advances in NMR methods and applications to materials* was organized in Bled, Slovenia between 18th and 22nd of September 2025.

In recent years, organization of the workshop rotates among Hirschegg (Austria), Cluj-Napoca (Romania), Debrecen (Hungary) and Bled (Slovenia). By tradition, it was held this year in Bled in the Plemljeva villa.

The abstract book is a collection of 20 abstracts of the presentations given at the workshop. These cover different fields of materials research by NMR spectroscopy and imaging and are categorized in five different sections: Porous materials, Polymers, Unusual NMR, Materials, Imaging, and Cements.

The meeting was organized by Igor Serša, Aleš Mohorič, Urška Mikac, and Rok Peklar.

A. Mohorič, I. Serša

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	9:30-10:00	Analysis of chemical exchange processes by NMR CPMG method Janez Stepišnik *University of Ljubljana, Ljubljana, Slovenia*
	10:00-10:30	Dynamics of binary fluids in porous media Niklas Siebert *Ilmenau University of Technology, Ilmenau, Germany*
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Polymers	11:00-11:30	Self-diffusion in (bi)disperse and uniform polyethylene oxide melts Kevin Lindt *Ilmenau University of Technology, Ilmenau, Germany*
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Session	Time	Lecture
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	12:00-12:30	Carbon black concentration effects in fresh and hardened cement paste: an NMR investigation Karoly Mostis *Technical University of Cluj-Napoca, Cluj-Napoca, Romania*
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	15:00-15:30	Magnetic resonance microscopy of coffee bean roasting Urša Mikac *Jožef Stefan Institute, Ljubljana, Slovenia*

	15:30-16:00	Coffee break
Imaging II	16:00-16:30	Feasibility of MRI using straight wires as coils for spatial signal encoding Kaja Tušar *COSYLAB, Ljubljana, Slovenia*
	16:30-17:00	Investigating dendritic growth in symmetrical lithium cells through MRI and simulation Rok Peklar *Jožef Stefan Institute, Ljubljana, Slovenia*

ABSTRACTS

Exchange Dynamics and Relaxation in Poymers Systems Studied by NMR

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Understanding the behavior of ionic solvents like ionic liquids (ILs) within polymer matrices is essential for advancing applications in energy storage, soft electronics, and responsive materials. In this study, we investigate the molecular dynamics of ILs confined in host polymer systems with varying degrees of rigidity. Two distinct regimes are explored: (i) rigid polymer matrices, where ILs remain phase-separated and the polymer acts as a porous scaffold, and (ii) soft polymer matrices, where ILs and polymers form a gel-like composite through partial mixing. Using a combination of Nuclear Magnetic Resonance (NMR) and Electron Paramagnetic Resonance (EPR) spectroscopy, we probe the mobility and local interactions of IL molecules across these environments. Our analysis reveals that ILs exhibit higher mobility within rigid matrices compared to soft ones. This behavior is interpreted through models based on dipolar and exchange interactions between free electrons in embedded radicals, offering insight into the microscopic mechanisms governing IL dynamics under confinement. These findings highlight the critical role of matrix rigidity in tuning ionic mobility, with implications for the design of functional polymer–IL hybrid systems.

ANALYSIS OF CHEMICAL EXCHANGE PROCESSES BY NMR CPMG METHOD

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The NMR CPMG method will be shown, with which we can effectively capture the spectrum of molecular conformation fluctuations caused by chemical exchange processes or other chemical reactions. The decay of the CPMG spin echo peaks yields an effective spin-relaxation time, which is directly related to the spectral density of the chemical exchange rate at the modulation frequency defined by the pulse repetition interval. The experimental results on sucrose–water mixtures are well described using chemical Langevin equations [1], suggesting that the observed frequency dependence of the fluctuation spectrums more accurately characterized by a cascading series of potential barriers rather than a single barrier as shown in attached figures. These findings deepen our understanding of the relationship between molecular dynamics and NMR relaxation phenomena and open new avenues for investigating complex exchange processes in multi-state systems.

[1] D.T. Gillespie, The chemical Langevin equation, J. Chem Phys.113 (2000) 297.

Dynamics of binary fluids in porous material

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Several binary liquids were prepared with different mixing ratios in equal steps of 10 vol-%. All mixtures were prepared with a protonated and a deuterated liquid to simplify data analysis. The relaxation times and the diffusion coefficient of the protonated liquid were measured at a Larmor frequency of 42,6 MHz and 300 K in the bulk phase and filling the pore space of Vycor. Mesoporous Vycor glass has a mean pore diameter of 4 nm with a high specific surface area. The ratio of the relaxation times between Bulk and Vycor represents the interaction between the molecules and the pore surface, which is covered with polar and protic hydroxyl groups. Mixtures with a nonpolar liquid like cyclohexane show an almost negligible interaction with the surface, while polar molecules have a significantly higher surface affinity due to adsorption. The ratio of the diffusion coefficient between bulk and Vycor describes the apparent tortuosity. The apparent tortuosity of Vycor is well known and in the range of 5 to 7 for pure liquids [1]. A concentration dependence and an increase of the apparent tortuosity in the Vycor indicate concentration gradients inside the pore space, suggesting demixing or partial phase separation. The molecules with a higher surface affinity (regarding to the relaxation times) also exhibit a higher apparent tortuosity which was found for acetone in cyclohexane and water in acetone. Only for binary mixtures of acetone and THF a constant apparent tortuosity of 6 could be found.

[1] S. Stapf et al., Magn. Reson. Lett. 3, 108 (2023)

Self-diffusion in (bi)disperse and uniform polyethylene oxide melts

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The self-diffusion in polymer melts depends on various parameters, such as the molar mass, the presence of entanglements, or the chain rigidity. Common to the majority of models and studies investigating the dynamics in polymer melts is the restriction to ideal, uniform linear molecules with a well-defined length, a situation that is never perfectly met in real polymers. In this contribution we investigate the relative change of diffusion properties in bidisperse polyethylene oxide (PEO) melts, i.e., uniform chains (10% ^{1}H PEO) in a matrix of shorter or longer uniform chains (90% ^{2}H PEO), in comparison to the diffusion behavior in uniform melts (100% ^{1}H PEO, dispersity of typically 1.1 or better). Furthermore, we explore the influence of dispersity (M_w/M_n) on diffusion by comparing a uniform bulk sample with a disperse blend of similar M_w. The measurements were carried out on the ^{1}H resonance using a Bruker Diffusion Observe Broadband Probe (g_{max} = 17 or 29 T/m, ν = 500 MHz) at variable temperatures above the bulk melting point of PEO between 343 K and 373 K. The presence of the dominant ^{2}H matrix clearly affects the mobility of the minority ^{1}H chains, while only a subtle influence of dispersity is observed. However, the quantification of diffusion coefficients, and therefore the assessment of differences, remains challenging due to significant deviations from simple Gaussian diffusion decays, not only in disperse blends but also in uniform bulk.

Swelling kinetics and structure of biodegradable crosslinked polyurethanes by NMR

M. Kéri[1], V. Papp[1] and I. Bányai[1]
[1]*University of Debrecen, Dep. of Phys. Chemistry, 4032, Debrecen, Egyetem tér 1., Hungary*

Biocompatible and biodegradable polymers are popular nowadays due to the growing demand of medicine, pharmacy, and environmental protection. Crosslinked polymer networks are usually tested by their thermal, mechanical, and swelling properties; however, liquid phase NMR spectroscopy is an appropriate complementary technique.[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. 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. By this novel approach in the description of swelling kinetics a second-order kinetic mechanism was found in DMSO. 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.
[1] Besghini, D.; Mauri, M.; Simonutti, R., Applied Sciences vol. 9(9) (2019) 1801.

Relaxivity properties of paramagnetic metal ion complexes with polymers prepared either with thermal condensation or assembled from smaller building blocks

L. Novák[1], I. Bányai[1], X. Feng[1], J. Lőrinczi[1]
[1]*University of Debrecen, Faculty of Science and Technology, Dept. of Physical Chemistry,*

Paramagnetic metal chelates of macromolecules can take advantage of a much longer rotational correlation time than complexes prepared from small molecules, therefore at the same metal ion concentration, they permit to attain significantly shorter T1 and T2 proton relaxation times in aqueous solutions. On the other hand, such polyionic molecules can also be used for heavy metal ion removal from solution. The synthesis of the macromolecular ligands consists generally in grafting well-characterized small chelators onto large polymers used as platforms. It is much less common to start the synthesis from "generic" macromolecules, since the characterization of the resulting products is not as easy. As a continuation of our previous work, we tried to follow two new methods of synthesis. The first one still consists in the functionalization of a macromolecule, this time polyacrylic acid, but using an uncommon method: direct thermal condensation with different amines in a polar aprotic medium, without using any activator or catalyst. Our second method uses small molecules as building blocks instead, these building blocks can then freely be combined with each other to yield different chelating polymers. We present here some preliminary results obtained with Cu(II) and Mn(II) complexes of the polyacrylate-based macroligands and with Gd(III) complexes of those synthesized from smaller building blocks.

To boldly go where no NMR has gone before: discovering new planets

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The existence of extraterrestrial planets has been suggested, predicted, or expected for centuries, with arguments that were more or less convincing and based on physical reasoning. However, the eventual discovery of planet-like stellar satellites in the 2nd half of the 20th century represented a paradigm change: finally there was hard proof for these expected planetary bodies, opening up scientific, philosophical and theological discussions. Somewhat surprisingly, three of the four most important detection methods are understood on the level of school physics, but no discovery had been reported due mostly to the limited instrumental sensitivity and a lack of analytic software.

This presentation introduces the main contemporary detection methods, statistical treatment of the results, and selected findings that constitute the current knowledge about extrasolar planets and bodies. This presentation is guaranteed not to contain any traces of NMR or EPR.

Signal Enhancement in Quadrupole Resonance

T. Apih
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Nuclear quadrupole resonance (NQR) can be thought of as NMR in solids, but without an external magnetic field. Instead of Zeeman interaction, the resonance frequency is determined by the interaction of $(I > 1/2)$ nuclear quadrupole moment with the gradient of electric field at the site of the nucleus. Since there is no preferred orientation in space, the NQR spectra of monokristalu and powders are exactly the same with no broadening of the resonance lines. This fact makes especially ^{14}N NQR very useful for the analysis and quality control of active pharmaceutical ingredients[1], which are more difficult to solve with other methods. The main drawback of ^{14}N NQR is low sensitivity, related mainly with low MHz frequency range of the resonances lines. We explore some old[2], some recent, and propose some new methods to enhance the NQR signals and make the method useful in for broader range of substances.

[1] Z. Trontelj, J. Pirnat, V. Jazbinšek, J. Lužnik, S. Srčič, Z. Lavrič, S. Beguš, T. Apih, V. Žagar, and J. Seliger, 2020. Nuclear quadrupole resonance (NQR) - a useful spectroscopic tool in pharmacy for the study of polymorphism. *Crystals*, *10*(6) p.450.
[2] J. Seliger, V. Žagar. New Methods for Detection of ^{14}N NQR Frequencies. *Appl Magn Reson* **43**, 469–484 (2012)

NMR around the radioactive waste repository

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The application of multi-barrier systems in radioactive waste repositories is crucial. The comprehensive characterization of each level of the multi-barrier system is required from the viewpoint of the potential migration of radionuclides from the repository. [1] The typical components of the barrier system are the solidified waste form, the waste container, the buffer/ backfilling materials and the host rock. [1] The structure and aqueous behavior of the different levels of a multi-barrier system (model cemented waste packages, bentonites, Boda Claystone Formation) were investigated by the combination of mainly low- and high-field NMR techniques and leaching studies. Our aim was to describe the diffusivity of water within the individual barriers as well as to gain insight into the properties of the barriers which may affect the mobility of water (e.g.: swelling, permeability, $T_{2cut\text{-}off}$) and the leaching behavior of the waste packages upon interaction with water. [2-4]

[1] Ojovan, M. I., et al., *An Introduction to Nuclear Waste Immobilisation*. Elsevier: **2019,** pp. 415.
[2] Papp, V., et al., *The Journal of Physical Chemistry B* **2025,** *129* (22), 5607.
[3] Fleury, M., et al., *Magn Reson Imaging* **2019,** *56*, 32.
[4] Testamanti, M. N., et al., *Journal of Petroleum Science and Engineering* **2017**, *149*, 497.

Relaxation spectra of variable pH water

Aleš Mohorič[1,2] and Jan Jamnik[1,2]
[1]Faculty of mathematics and physics, University of Ljubljana, Ljubljana, Slovenia, [2]Jožef Stefan Institute, Ljubljana, Slovenia

NMR relaxation measurements offer a window into water's hydrogen-bond network and proton exchange dynamics. pH variations shift equilibria among H_3O^+, H_2O, and OH^-, altering motional regimes. We investigate transverse relaxation dispersion across pH 2–12 with CPMG sequence with variable interpulse spacing to measure frequency-dependent transverse relaxation rates to elucidate how acid—base conditions reshape water's dynamic architecture at the microscopic scale. Dispersion profiles exhibit pronounced low-frequency curvature at extreme pH and flattened behavior near neutrality. Fitting these curves with molecular conformation fluctuation spectrum formalism yields same high-frequency offsets, different dispersion amplitudes, cutoff frequencies and stretching exponents that quantitatively describe motional distributions. Results indicate that extreme acidic and alkaline environments enhance slow, exchange-dominated fluctuations, manifested as elevated amplitudes and reduced cutoff frequencies while neutral water shows minimal dispersion, reflecting uniform rapid motions.

[1] Meiboom S., Gill D. Modified spin-echo method for measuring nuclear relaxation times. Rev. Sci. Instrum. 1958;29(8):688–691. https://doi.org/10.1063/1.1716296
[6] Stepišnik J., Mohorič A. Chemical Exchange Rate Study by NMR CPMG Method. Applied Magnetic Resonance 54, 1411–1422, (2023). https://doi.org/10.1007/s00723-023-01621-z

Microplastic in Sediments of the Skagerrak Depo Centre

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Microplastic is a pollutant that came into focus during the last decade. Huge amounts are expected to have entered the environment, but actual quantities, distributions and potential hazards are still mostly unknown. We present microplastic distribution data from sediment cores taken at the Skagerrak depo centre, an accumulation site for fine-grained sediments in the North Sea [1]. The microplastic composition was measured with two different spectroscopic methods, Raman spectroscopy and py-GC/MS, which enables us to compare the performance of these two techniques. The measured microplastic distribution was implemented into numerical transport reaction models. These models could successfully be used to extract crucial parameters for the assessment of environmental risks like particle input fluxes and distribution of harmful leachates from the microplastic particles.

[1] T. Spiegel et al., Frontiers in Marine Science, 10 (2023), 1141448.

A new multi-modal (x-ray) instrument for the study of functional materials

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Right now, the conversion from carbon-based energy sources to renewable energies is a major research topic and challenge. Many new materials are being synthesized with the aim to improve catalytic activity and selectivity, especially for photo- and electro-catalytic applications. The function of these materials depends on the size, long-range order, local structure, and oxidation state, and all these parameters can change under operando conditions. Therefore, it is essential to investigate these parameters on an atomic or molecular level under realistic operando conditions simultaneously in combination with macroscopic parameters, which characterize the function of the material. X-rays are perfectly suited to study the structure on a molecular/atomic level, since the wavelength of x-rays is of the order of inter-atormic distances. The electronic and geometric structure of materials are closely related, and they influence each other since the valence electrons have a direct impact on both structures. The new instrument [1] at the synchrotron raditation source PETRA III is dedicated to combine x-ray diffraction and x-ray absorption measurements in order to get information on the electronic and local structure, and long range order simultaneously.

[1] WA Caliebe, A Kalinko, M Viehweger, S Pfeffer, J Horbach, M Görlitz, Sergey Peredkov, Arno Bergmann, Janis Timoshenko, Journal of Physics: Conference Series, 2025, Vol. 3010, p. 012168

Synthesis and characterisation of carbon aerogels doped with graphene.

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Carbon based porous gels are widely used in battery and supercapacitor industry. Graphene based electrode materials have promising properties, like more flexible 3D skeleton, better electrical conductivity and higher resistance against oxidation. Sadly, producing graphene based electrodes at industrial scale is a hard task. Therefor we would like to make electrochemically active cathode materials by adding graphene oxide as a dopant during the synthesis of resorcinol-formaldehyde based aerogels. NMR cryoporometry and NMR relaxometry are widely used for measuring pore size distribution and surface interactions. By measuring freezing and melting point depression in fully saturated pores we can determine the pore shape and pore size distribution. The evolution of relaxation time constants during saturation can give us further information from the surface of the carbon material, like hydrophilicity and distribution of hydrophilic regions inside the material.

FFC NMR relaxometry studies of carbon modified cementitious composites

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Additive manufacturing with cement-based materials offers promising pathways for reducing the environmental impact of the construction sector. Moreover, the integration of carbon-based conductive additives into cementitious composites enables the development of multifunctional materials with applications such as self-heating, structural health monitoring, and energy harvesting. Consequently, this study presents an interdisciplinary approach combining 3D printing technology with carbon-modified cement composites. Carbon black is pre-dispersed in aqueous superplasticizer solutions to enhance dispersion and minimize exposure risks. The influence of water content on the fresh and hardened properties of the paste is investigated using Fast Field Cycling NMR relaxometry techniques. The evolution of surface affinity and surface-to-volume ratio during hydration is evaluated and correlated with complementary techniques to assess the extrudability and buildability of the resulting systems. *ACKNOWLEDGEMENT*: This research was funded by a grant of the Romanian Ministry of Education and Research, CNCS—UEFISCDI, Project Number 27/01-07-2024, within program GCNAC ARUT 2023. I.A. acknowledges the support received through a grant from the Ministry of Research, Innovation and Digitization, CNCS/CCCDI - UEFISCDI, project number ERANET-M3-STF4SW, within PNCDI IV.

Evaluating the printability of carbon modified cementitious composites

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Carbon-modified cementitious composites emerge as multifunctional materials with promising applications such as self-heating, structural health monitoring, energy harvesting, and improved mechanical or durability performance. The current study explores such composites in the context of additive manufacturing with cement-based materials. Carbon black powder is pre-dispersed in superplasticizer-based aqueous solutions to enhance dispersion and homogeneity in the final cement paste. NMR relaxometry techniques are used to monitor the effects of water content—both in carbon dispersions and in composite paste, to further aid in the mortar classification as printable or non-printable [1]. The results are compared with complementary techniques to establish how certain morphological and structural features of carbon modified cementitious pastes impact their performance.

ACKNOWLEDGEMENT: This research was funded by a grant of the Romanian Ministry of Education and Research, CNCS—UEFISCDI, Project Number 27/01-07-2024 and 7/01-07-2024, within program GCNAC ARUT 2023. I.A. acknowledges the support received through a grant from the Ministry of Research, Innovation and Digitization, CNCS/CCCDI - UEFISCDI, project number ERANET-M3-STF4SW, within PNCDI IV.

[1] M. M. Rusu and I. Ardelean, *Materials*, vol. 18, no. 13, p. 3070, Jun. 2025, doi: 10.3390/ma18133070.

Carbon Black Concentration Effects in Fresh and Hardened Cement Paste: An NMR Investigation

Karoly Mostis[1], Mihai M. Rusu[1], Ioan Ardelean[1]
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This study investigates the influence of carbon black (CB) concentration on the hydration and pore structure of cement paste using nuclear magnetic resonance (NMR) relaxometry. Three systems with CB between 0% and 10% additions were analyzed in both fresh and hardened states. The hydration process and cyclohexane desorption kinetics were monitored using NMR-CPMG measurements. The dependence of the relaxation rate and filling factor (A/A_0) during desorption processes on the hardened samples is discussed.

Artificial Intelligence in the Optimization of Inversion RF Pulses

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Experimental conditions are often such that the homogeneity of the static magnetic field B_0 and/or the RF magnetic field B_1 is poor. In these cases, the performance of most RF pulses is suboptimal and usually results in MR images with artifacts. In this study, we demonstrate that artificial intelligence can be used to mitigate this problem by helping to find the most optimal RF pulses for given experimental conditions, e.g. RF pulses can be optimized to tolerate larger B_0 or B_1 inhomogeneities, or both, than their conventional counterparts. Specifically, we tested the performance of different inversion RF pulses, adiabatic and AI-generated, with a magnetization prepared rapid acquisition gradient echo (MP-RAGE) sequence on two test samples: a 3D-printed plastic container filled with agarose and a biological sample. In the case of both samples, the B_0 homogeneity was intentionally spoiled in some spots by metallic inclusions or tiny ferromagnetic fragments, while the influence of B_1 on the image was tested using RF transmitter/receiver probes with different B_1 homogeneities. The obtained preliminary results indicate the superiority of AI-generated inversion pulses compared to conventional RF pulses and thus encourage us to expand the current study to other types of pulses used in other imaging pulse sequences.

[1] V.S. Manu, C. Olivieri, G. Veglia, Nat. Commun. (2023)14:4144.

Magnetic resonance microscopy of coffee bean roasting

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Coffee is one of the most beloved beverages in the world, known for its rich aroma, bold flavor, and energizing effect. Coffee's character comes not just from the bean itself, but from how it's roasted. Roasting is a crucial step in the coffee-making process. It transforms the green, raw coffee beans into the dark, aromatic beans we recognize. During roasting, heat triggers complex chemical reactions that develop the flavors, acidity, aroma, and body of the coffee. A light roast might preserve more of the bean's original, fruity notes, while a dark roast brings out deeper, smokier flavors. Lipids, though present in relatively small amounts in coffee beans (about 10–16% of the bean's dry weight), play an important role in the quality, flavor, and overall coffee experience. During the roasting process, the expansion of coffee beans causes structural changes that result in the oleosome destruction and the migration of lipids toward the bean's surface [1]. In this study, MRI was used to monitor the migration of lipids during roasting process.

[1] K. Williamson, E. Hatzakis, Food Chemistry 299 (2019) 125039.

Feasibility of MRI using straight wires as coils for spatial signal encoding

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[1]*Jožef Stefan International Postgraduate School, Ljubljana, Slovenia*
[2]*Jožef Stefan Institute, Ljubljana, Slovenia*

In this talk, I will present recent work on exploiting a simple straight wire segment as the fundamental building block for generating highly nonlinear magnetic fields, with applications in magnetic resonance imaging and advanced field encoding. After a brief introduction to the theory of image reconstruction, I will describe the design of the coils and the experimental setup used to characterize their behavior. A series of illustrative measurements—including results on carrot, strawberry, and two dedicated test samples—will demonstrate the feasibility and sensitivity of this approach. Finally, I will extend the discussion to the theoretical framework for three-dimensional coils and highlight two possible coil arrangements capable of achieving full 3D encoding. Together, these results suggest a versatile and scalable methodology for constructing compact, nonlinear field sources from the simplest current-carrying elements.

Investigating Dendritic Growth in Symmetrical Lithium Cells through MRI and Simulation

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Li-metal batteries promise high energy, but dendrites limit safety and life. This work couples operando MRI with stochastic growth models to identify where dendrites nucleate, how they propagate, and how circuitry and transport affect morphology. We build MRI-compatible symmetric Li cells and image deposition in 3D, resolving electrolyte-depletion fronts, gas formation, and electrically isolated "dead Li." A topology study shows parallel-wired compartments concentrate current and trigger runaway filaments, whereas series connection enforces more uniform, planar growth. We implement an electric-field-biased 3D DLA (with Laplace potential) and a 2D multi-body DLA that map the roles of ion supply, interfacial kinetics, and bias in transitions from sparse fractals to compact deposits. Together, MRI and modelling support an electrochemomechanical picture: concentration gradients and current-density heterogeneity set growth regimes [1,2]. The results support mitigation strategies that homogenize current and promotes ion transport.

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