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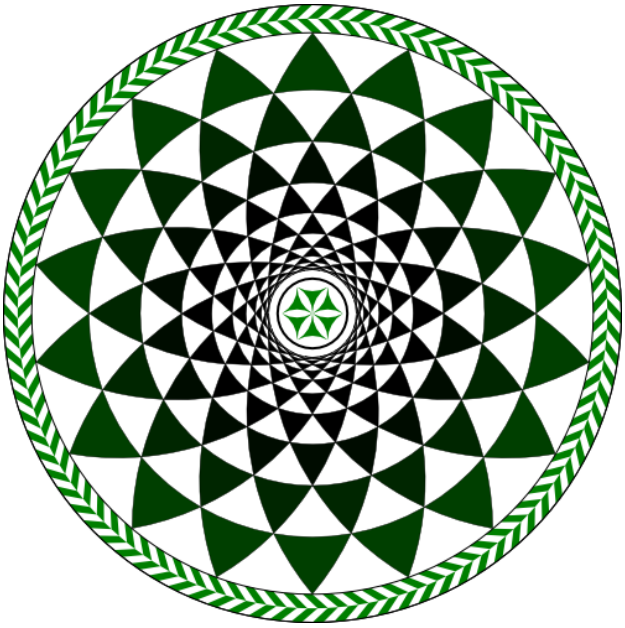

Multiscale Phenomena in Condensed Matter

7 – 10 July 2026

THE HENRYK NIEWODNICZAŃSKI
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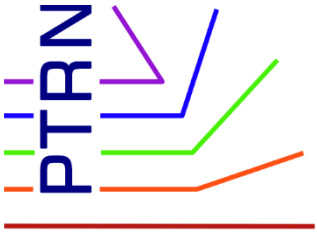

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PRESENTATIONS

Tuesday, 7 July 2026

Opening lecture

15:30-16:30 **Eric Collet** (Rennes, France)

From ultrafast photoinduced charge-transfer polarons to macroscopic phase transition

II. Molecular magnets and nanomagnets (a)

16:30-17:05 **Konrad Cyprych** (Wrocław, Poland)

Multiscale phenomena in light-matter interactions

17:05-17:35 **Erik Čižmár** (Košice, Slovakia)

Cluster spin glass in Co-Al and Ni-Fe layered double hydroxides

17:35-18:05 **Marek Pasciak** (Prague, Czech Republic)

Sub-THz dynamics in (anti)ferroelectrics: from overdamped soft modes to polar skyrmions

18:05-18:35 **Dawid Pinkowicz** (Kraków, Poland)

Photomagnetic switching in heavy cyanometallates: light-induced excited spin state trapping or cyanide photodissociation?

Wednesday, 8 July 2026

I. Soft matter and glass formers (a)

08:30-09:05 **Frank Schreiber** (Tübingen, Germany)

Multiscale behavior in soft matter: From phase diagrams to dynamics

09:05-09:35 **Daria Szewczyk** (Wrocław, Poland)

From molecular geometry to glassy response in benzene-based crystals

09:35-10:05 **Francesca Nardelli** (Pisa, Italy)

Probing polymer and water dynamics in anion exchange membranes by solid-state NMR spectroscopy

10:05-10:35 **Oleksandr Kryvchikov** (Kharkiv, Ukraine)

Origin of the linear heat-capacity term in Graphite-Based Nanomaterials

I. Soft matter and glass formers (b)

11:05-11:40 **Simone Simon Napolitano** (Brussels, Belgium)

Tiny movements, big change: when collective small displacements control flow and aging in soft matter

11:40-12:10 **Hal Suzuki** (Osaka, Japan)

Calorimetric studies on melting of rubbers under strain

12:10-12:40 **Daniele Sonaglioni** (Pisa, Italy)

Acceleration of the crystal growth across the liquid to glass transition

12:40-13:10 **Francesca Martini** (Pisa, Italy)

Probing structure and dynamics in functional porous materials by solid state NMR spectroscopy

IV. Spectroscopic methods in materials research (a)

14:10-14:45 **Marco Geppi** (Pisa, Italy)

NMR and NQR of functional materials for environmental, energy, and optoelectronic technologies

14:45-15:15 **Yasuhiro Nakazawa** (Osaka, Japan)

Electron correlation induced glasses in molecular compounds

15:15-15:45 **Anatoli Serghei** (Villeurbanne, France)

Scaling laws of electrical conductivity in conductive materials: length-scale and universality

15:45-16:15 **Arthur Markus Anton** (Leipzig, Germany)

Identifying molecular moieties incorporated in charge transport and their contribution to conductivity

16:15-16:45 **Alicia Forment-Aliaga** (Valencia, Spain)

Chemically modified 2D materials: Unlocking new properties and functionalities

Thursday, 9 July 2026

V. Computational physics, modeling, and machine-learning approaches (a)

08:30-09:00 **Konrad Kapcia** (Poznań, Poland)

Landscape of ordered phases in a localized-fermion system with on-site and intersite interactions on a triangular lattice

09:00-09:30 **Paweł Karbowniczek** (Kraków, Poland)

Generalized Landau–de Gennes theory of polar and modulated nematic phases

09:30-10:00 **Zita Tokárová** (Trnava, Slovakia)

Correlating experimental and DFT electronic structures of organic dopants for OLED materials

10:00-10:30 **Radosław Strzałka** (Kraków, Poland)

Research on Bergman-type quasicrystals: disorder and stability

III. Neutron and X-ray scattering methods (a)

11:00-11:35 **Mark Johnson** (Grenoble, France)

Institute Laue-Langevin - instrument and infrastructure upgrades, the science strategy and new research opportunities for Poland

11:35-12:05 **Giovanna Costa** (Bauru, Brasil)

Solid-state study of a new venlafaxine and catechol cocrystal

12:05-12:35 **Cheuk-Wai Tai** (Stockholm, Sweden)

Study of imperfect structure in materials by Electron Diffraction

12:35-13:05 **Maths Karlsson** (Göteborg, Sweden)

Local structure and dynamics in halide perovskites investigated with inelastic neutron scattering

13:05-13:35 **Regina Stachura** (Kielce, Poland)

Analysis of Ti and TiO_2 nanolayers irradiated with HCI X^{eq+} using SR-GIXRF and SR-XRR methods

VI. Multifunctional, ferroelectric, and multiferroic materials (+ Soft matter)

14:35-15:10 **Denys Makarov** (Dresden, Germany)

Curvilinear electronics: from geometry-induced magnetochirality to efficient THz converters

15:10-15:40 **Marian Paluch** (Chorzów, Poland)

Enhancing the physical stability of amorphous pharmaceuticals through control of molecular mobility

15:40-16:10 **Żaneta Wojnarowska** (Chorzów, Poland)

Decoupling between the structural and conductivity relaxation as a fingerprint of the ion transport mechanism

16:10-16:40 **Krzysztof Wojciechowski** (Kraków, Poland)

Attuned Electronic Structure–Mismatched Phonon Structure (AES–MPS): A unified framework for engineering the electronic–phonon transport in thermoelectric materials

Friday, 10 July 2026

VI. Multifunctional, ferroelectric, and multiferroic materials (b)

08:30-09:05 **Damian Rybicki** (Kraków, Poland)

Studies of magnetic properties of Eu compounds

09:05-09:35 **Mateusz Mrukiewicz** (Warsaw, Poland)

Understanding electric permittivity behavior in highly polar liquid crystal systems

09:35-10:05 **Vladimir Lipp** (Schenefeld, Germany)

Submicron-precision machining of silicon surface with intense femtosecond extreme ultraviolet pulses

10:05-10:35 **Samuel Mañas-Valero** (Valencia, Spain)

Visualizing spin waves with color center magnetometry

VI. Multifunctional, ferroelectric, and multiferroic materials (c)

11:05-11:35 **Monika Marzec** (Kraków, Poland)

Properties of DNA – surfactant complexes in thin films and bulk

11:35-12:05 **Vitalii Boiko** (Wrocław, Poland)

Role of the transition metals in persistent luminescence phenomena

12:05-12:35 **Marian Mihalik** (Košice, Slovakia)

Magnetocaloric effect in selected compounds with perovskite structure

12:35-12:50 **Michał Krupiński** (Kraków, Poland)

Confinement driven non-collinear spin-textures in embedded nanomagnets

II. Molecular magnets and nanomagnets (b)

14:00-14:30 **Lech Sznitko** (Wroclaw, Poland)

Exploring photonic applications of luminescent electrospun polymeric fibers

14:30-15:00 **Paul Kögerler** (Aachen, Germany)

Spintronic effects of chemisorbed aromatic cyclophanes

15:00-15:30 **Michał Rams** (Kraków, Poland)

Magnetic relaxation and ordering in single crystals of quasi-one dimensional $Co(NCS)_2(ligand)_2$ compounds

15:30-16:00 **Paweł Oświęcimka** (Kraków, Poland)

Multifractal characteristics of liquid crystal textures

16:00-16:15 **Piotr Zieliński** (Kraków, Poland)

Symmetric and 2D-chiral hinged gratings: geometric limits, robust self-similarity and generalized conformability

From ultrafast photoinduced charge-transfer polarons to macroscopic phase transition

M. Hervé[1,2], G. Privault[1,2], S. Zerdane[3], S. Akagi[4], S.-i. Ohkoshi[2,5], H. Tokoro[2,4], M. Cammarata[6], E. Collet[1,2,7]

[1] Univ Rennes, CNRS, Institut de Physique de Rennes, Rennes, France
[2] CNRS, Univ Rennes, DYNACOM – IRL 2015, The University of Tokyo, Japan
[3] Paul Scherrer Institute; Villigen, Switzerland
[4] Department of Materials Science, University of Tsukuba, Japan
[5] Department of Chemistry, The University of Tokyo, Japan
[6] ESRF – The European Synchrotron; Grenoble, France
[7] Institut Universitaire de France (IUF), France

Ultrafast control of functional materials by light is key for developing optoelectronic devices. Still, the mechanisms by which microscopic photoinduced excitations evolve into a macroscopic phase transformation remain poorly understood, partly due to the experimental challenges of isolating the multiscale electronic and structural dynamics. Here, we use femtosecond optical, infrared and X-ray techniques to track the non-equilibrium dynamics leading to macroscopic transformation in a ferroelastic charge-transfer Mn-Fe Prussian Blue analogue [1,2,3]. The experimental data evidence a sequence of phenomena from the ground Mn3+Fe2+ state to the photoinduced Mn2+Fe3+ state. The initial electronic excitation leads to reverse Jahn-Teller distortion on the Mn site within 50 femtoseconds, causing intermetallic charge-transfer polarons within 200 femtoseconds. Polarons generate significant lattice strain and trigger the phase nucleation within 60 picoseconds. This elastically-driven cooperativity towards the Mn2+Fe3+ phase, launched by the photoinduced polarons, offers an efficient route to the generation and stabilization of photoinduced phases in many volume-changing materials such as Prussian Blue analogues or spin crossover materials.

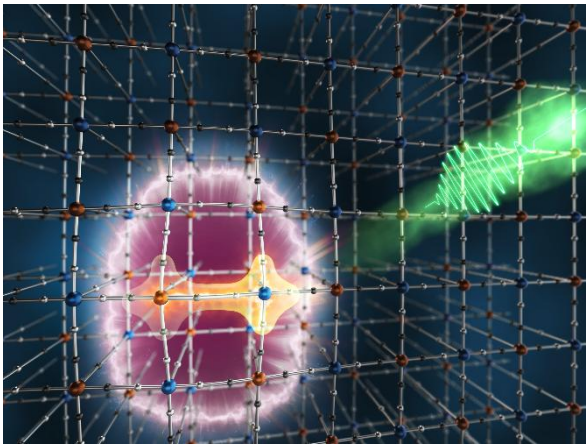

Figure 1. Ultrafast formation of a photoinduced charge-transfer polaron.

References:
[1] M. Hervé et al, *Nature Mater.*, 25, (2026), 588-594
[2] G. Privault et al, *Angew. Chem. I.E.*, 63, (2024), e202408284
[3] M. Hervé et al, *Nature Commun.*, 15, (2024), 267

Multiscale phenomena in light-matter interactions

K. Cyprych[1]

[1] Wroclaw University of Science and Technology, 27 Wybrzeże Stanisława Wyspiańskiego st., 50-370 Wroclaw, Poland, Faculty of Chemistry, konrad.cyprych@pwr.edu.pl

The control of light-matter interactions in condensed matter requires a sophisticated understanding of multiscale phenomena, spanning from molecular dynamics to macroscopic optical responses. This work explores the design and characterization of complex photonic systems using Two-Photon Polymerization (2PP) and natural biopolymeric architectures, applied in light amplification [1]. We applied Reaction Diffusion System (RDS) into 2PP as a source of designed randomness, possessing multiscale spatial alignment, similar to the 2PP process itself governed by reaction-diffusion systems, where the nonlinear interplay between radical generation, diffusion, and quenching determines the final voxel geometry and structural resolution. Utilization of these reaction diffusion dynamics, we fabricate hierarchical 3D photonic crystals.

Particular emphasis is placed on light amplification within these dielectric frameworks. By integrating gain media, we investigate the transition from spontaneous emission to lasing, driven by slow-light effects at the photonic band edges. We extend this multiscale approach to natural systems, specifically starch granules, which serve as unique anisotropic multiresonator platforms. Utilizing hyperspectral imaging with sub-micrometer resolution, we map the spatial distribution of lasing pathways within these granules. The results reveal that the internal "blocklet" architecture and radial birefringence of starch create a complex network of coupled resonators, acting as multiscale system. By applying Fourier transform analysis to the emission spectra, we identify dominant cavity modes correlated with the granule's structural heterogeneity [2]. This comparative study between synthetic 2PP structures and natural biopolymers highlights the universal role of multiscale hierarchy in optimizing gain dynamics and threshold conditions for the next generation of integrated photonic devices.

References:
[1] K. Piskorz et al., *Adv. Funct. Mater.*, 36, (2026), e16241
[2] K. Cyprych, M. Janeczko, J. Myśliwiec, *J. Opt. Soc. Am. B*, 42, (2025), 1457-1463

Cluster spin glass in Co-Al and Ni-Fe layered double hydroxides

E. Čižmár[1], V. Tkáč[1], E.L. Fertman[2], A.V. Fedorchenko[2], M. Holub[3], R. Tarasenko[1], Yu.G. Pashkevich[3], C.S. Neves[5], and A.N. Salak[5]

[1] Institute of Physics, Faculty of Science, P.J. Šafárik University in Košice, 04154 Košice, Slovakia, erik.cizmar@upjs.sk
[2] B. Verkin Institute for Low Temperature Physics and Engineering of NASU, 61103 Kharkiv, Ukraine
[3] Faculty of Physics and Applied Computer Science, AGH University of Krakow, 30059 Kraków, Poland
[4] O. Galkin Donetsk Institute for Physics and Engineering of NASU, 03028 Kyiv, Ukraine
[5] Department of Materials and Ceramics Engineering, CICECO – Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal

Frequency-dependent magnetic behaviour of Co-Al layered double hydroxides (LDH) with the Co/Al ratio (n) of 2 and 3, and the basal spacing values in the range of 0.76-1.66 nm was studied in detail between 2 and 300 K. It was found from analysis of the temperature-dependent *ac* magnetic susceptibility measured at different frequencies that the studied LDH exhibit a magnetic cluster spin glass (spin glass-like) behaviour regardless of their basal spacing value and the Co/Al ratio as evidenced by $E_A/k_BT_0 > 1$ relation as obtained from the analysis using Vogel-Fulcher law [1]. The obtained values of Mydosh parameters in the range of 0.017-0.052 suggest that some of these materials are not far from the canonical spin glasses, implying a rather small size of the magnetic clusters. In the case of Ni-Fe LDH, the glassy state is strongly dependent on morphology of crystallites, but it appears at higher temperatures and allows for the observation of aging and rejuvenation effects. The specific heat of non-magnetic Mg-Al LDH analogs at low temperatures revealed their 2D solid and structural glass character [2]. The reduced $C(T)/T^3$ of Mg-Al LDH intercalated with nitrate was found to demonstrate a so-called boson peak, which is a manifestation of a glassy state. The observed low-temperature structural glassy state in LDH was associated with the disorder of the intercalated species and can affect the creation of cluster spin glass in magnetic LDH.

Acknowledgements: The work was supported by the projects APVV-22-0172 and APVV-23-0006, and EU H2020 project European Microkelvin Platform (EMP), grant agreement No. 824109.

References:
[1] E.L. Fertman et al., *Chem. Phys. Lett.*, 859, (2025), 141745
[2] V. Tkáč et al., *Appl. Clay Sci.*, 266, (2025), 107695

Sub-THz dynamics in (anti)ferroelectrics: from overdamped soft modes to polar skyrmions

M. Paściak[1]

[1] Institute of Physics of the Czech Academy of Sciences, Na Slovance 2, 182 00 Prague, Czech Republic, pasciak@fzu.cz

The dynamics of ferroelectrics below the phonon frequency range is often governed by collective motion of local distortions and topological objects. These excitations frequently possess polar character, couple strongly to THz fields, and contribute significantly to dielectric response. Their characteristic time and length scales make them attractive for ultrafast, high-density information technologies.

In this talk I will present several examples of sub-THz dynamics in (anti)ferroelectrics studied experimentally and theoretically. In cubic $BaTiO_3$, diffuse scattering can be interpreted as overdamped soft-mode dynamics leading to short-lived polar chains [1]. In the antiferroelectrics $PbZrO_3$ and $NaNbO_3$, coupling to non-polar order parameters pushes whole branches of polar excitations to sub-THz regime. I will also discuss $PbTiO_3/SrTiO_3$ superlattices, where THz-field excitation and femtosecond x-ray diffraction reveal the dynamics of polar topological structures, including vortex tubes [2] and skyrmions [3].

The theoretical framework is based on first-principles-derived atomistic models. Harmonic excitations are obtained from dynamical-matrix calculations, while finite-temperature behavior is studied using molecular dynamics and analysis of the dynamical structure factor $S(q,\omega)$. Together, these approaches provide insight into sub-THz polar modes and their coupling to acoustic excitations and THz fields.

Acknowledgements: The research was supported by Czech Science Foundation Grant No. 25-15518L.

References:

[1] M. Paściak, T.R. Welberry, J. Kulda, S Leoni, and J Hlinka, *Phys. Rev. Lett.*, 120, (2018), 167601

[2] Q. Li, V.A. Stoica, M. Paściak, et al., *Nature*, 592, (2021), 376-380.

[3] H. Wang, V. Stoica, C. Dai, M. Paściak, et al., *Nature Commun.*, 16, (2025), 8994

Photomagnetic switching in heavy cyanometallates: light-induced excited spin state trapping or cyanide photodissociation?

D. Pinkowicz[1]

[1] Faculty of Chemistry, Jagiellonian University, Kraków, Poland,
dawid.pinkowicz@uj.edu.pl

Photomagnetism is an intrinsic property of several heavy cyanometallates and has been repeatedly exploited to achieve photomagnetic switching in various coordination compounds, including multinuclear molecules,[1] coordination chains[2] and three-dimensional coordination frameworks.[3] Over time, it became increasingly clear, that in most cases, the photoswitching of cyanometallates is associated with the reversible photodissociation of a cyanide ligand.[4,5] This mechanism was supported by several photodissociation studies in solution, including the successful isolation of relevant photoproducts.[4-6] Nevertheless, a few reports continued to suggest an alternative mechanism,[7] resembling light induced excited spin state trapping, LIESST.

Here, we present an unequivocal demonstration of an extremely clean LIESST-type effect in potassium octacyanoniobate(III), $K_5[Nb^{III}(CN)_8]$, representing the first structural example of a LIESST effect in a complex other than 3*d* transition metal.[8] Structural studies in the dark and at 30 K reveal, that the $[Nb^{III}(CN)_8]^{3-}$ complex anion adopts a nearly ideal dodecahedral geometry. Upon green light irradiation, however, it undergoes a strongly anisotropic geometrical distortion, involving pronounced elongation of the four Nb-C bonds aligned along its S_4 symmetry axis by nearly 0.2 Å, while the remaining four Nb-C bonds are slightly shortened. This unprecedented structural distortion is accompanied by a change in the effective magnetic moment from zero to 1.6 μ_B, suggesting a spin-state change from S = 0 to S = 1. All observed photo-induced changes are reversible by red light irradiation or heating above 50 K. Further details will be presented during the talk and compared with the opposite photoswitching mechanism: an extremely clean example of reversible cyanide photodissociation in $K_4[Mo^{III}(CN)_7]\cdot 2H_2O$.[5]

Acknowledgments: this work was financed by the European Union within the Horizon Europe Framework Programme, ERC Consolidator Grant LUX-INVENTA no. 101045004.

References:
[1] M. Arczyński et al., *J. Am. Chem. Soc.*, 141, (2019), 19076-19077
[2] M. Magott et al., *Angew. Chem. Int. Ed.*, 56, (2017), 13283-13287
[3] M. Magott et al., *J. Am. Chem. Soc.*, 140, (2018), 15876-15882
[4] X. Qi et al., *Angew. Chem. Int. Ed.*, 59, (2020), 3117-3121
[5] M. Magott et al., *Nat. Commun.*, 16, (2025), 8377
[6] M. Magott et al., *Chem. Commun.*, 57, (2021), 9926-9929
[7] N. Bridonneau et al., *Chem. Commun.*, 51, (2015), 8229-8232
[8] W. Wolański, J. Yadav, D. Pinkowicz et al., (2026), in preparation

Multiscale behavior in soft matter: From phase diagrams to dynamics

F. Schreiber[1]

[1] Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany, frank.schreiber@uni-tuebingen.de

It is established by now that for biomolecular systems not only the time-averaged structure is important, but also their dynamics. In particular proteins as the "machinery of life" have been subject of detailed investigations. In a simple approximation one may expect globular proteins to exhibit more or less simple Brownian motion and to be describable using concepts derived from colloid science. While this is not wrong, there are important refinements of this picture, and the spectrum of scenarios is rather broad due to effects such as

- crowding
- complex interactions
- multi-component solutions of more than one species
- non-sphericity of the proteins
- internal degrees of freedom
- association or aggregation in particular under high concentrations

In many cases, not only the behavior of individual proteins needs to be understood, but rather the collective phenomena, which remains a challenge, in particular quantitatively [1]. We discuss concepts for controlling and understanding protein phase diagrams, including aggregation pathways and the branching between them in aqueous solution by addition of multivalent ions or depletion agents. The tailoring of the interaction potential is exploited for controlling a) crystallization, b) gelation and amorphous aggregation, c) smaller aggregate formation, as well as d) network formation, with particular emphasis on kinetics and dynamics. We present complementary investigations of the dynamics of these systems using X-ray photon correlation spectroscopy (XPCS) and quasi-elastic neutron scattering (QENS), employing backscattering and spin-echo techniques [1-2]. We discuss how these can be exploited to address complex protein solutions under the conditions a) – d) above, including network formation in these systems and the associated dynamics on different time and length scales. We also comment on the relationship with theory and simulations and to which extent coarse-grained colloidal or polymeric models can be employed to describe proteins [2], in particular in view of their internal degrees of freedom and specific functionalities, as well as self-organization behavior [3]. Invaluable contributions by numerous collaborators are gratefully acknowledged as is financial support by ILL, EU, BMBF, DFG, and ANR.

References:

[1] M. Grimaldo et al., *Q. Rev. Biophys.*, 52, (2019), e7
[2] A. Girelli et al., *Nature Commun.*, 16, (2025), 10814
[3] L. Mateo Minarro et al., *PNAS*, 123, (2026), e2532636123

From molecular geometry to glassy response in benzene-based crystals

D. Szewczyk[1], A. Jeżowski[1], A.I. Krivchikov[1,2], M.A. Ramos[3], J. F. Gebbia[4], J.Ll. Tamarit[4]

[1.]Institute of Low Temperature & Structure Research PAS, Wrocław, Poland, d.szewczk@intibs.pl
[2.]Institute for Low Temperature Physics & Engineering NASU, Kharkiv, Ukraine
[3.]Universidad Autónoma de Madrid, Madrid, Spain
[4.]Universitat Politècnica de Catalunya, Barcelona, Catalonia, Spain

We investigate how microscopic substitution patterns in benzene derivatives propagate across length scales to shape emergent glassy excitations in quasiplanar molecular crystals. High-resolution heat-capacity measurements are reported for a series of compounds that systematically vary the number and spatial arrangement of methyl and chlorine substituents.

All systems exhibit canonical signatures of glassy behavior, including a linear term in the low-temperature heat capacity attributed to two-level systems (TLS) and a broad or smeared maximum in C_p/T^3 near ~10 K, consistent with a boson peak. By comparing molecules with controlled symmetry breaking—such as symmetric versus asymmetric methyl placement and distinct chlorine–methyl topologies—we resolve how subtle geometric modifications at the molecular scale influence the mesoscale landscape of low-energy excitations.

We find that the TLS density and the boson-peak characteristics (position and intensity) are governed not only by substituent count but critically by their spatial arrangement. In particular, configurations with equivalent versus inverse substitution patterns reveal that small changes in molecular asymmetry strongly perturb the distribution of local potential wells and coupling between librational and collective modes. This demonstrates that symmetry and local packing frustration, rather than overall orientational disorder alone, dominate the emergence of glassy anomalies.

Our results establish a clear link between substitution-driven molecular structure and collective vibrational response, providing experimental constraints for models of TLS formation and boson-peak origin in molecular crystals.

Probing polymer and water dynamics in anion exchange membranes by solid-state NMR spectroscopy

F. Nardelli[1,2,3], A. Giovanelli[1], S. Rotundo[1], M. Geppi[1,3], A. Pucci[1,3], F. Martini[1,3]

[1] Dipartimento di Chimica e Chimica Industriale, Università di Pisa, via G. Moruzzi 13, 56124, Pisa (Italy), francesca.nardelli@unipi.it
[2] Istituto di Chimica dei Composti Organo Metallici, Consiglio Nazionale delle Ricerche, via G. Moruzzi 1, 56124, Pisa (Italy)
[3] CISUP, Centro per l'Integrazione della Strumentazione dell'Università di Pisa, Lungarno Pacinotti 43, 56126, Pisa (Italy)

Solid-state NMR (SSNMR) spectroscopy is a powerful tool for investigating molecular structure, dynamics and host-guest interactions in functional polymeric membranes. By probing nuclear observables such as relaxation times and anisotropic line shapes, SSNMR can provide site- and phase-sensitive information on both the polymer matrix and absorbed guest molecules, offering molecular-level insight into properties that are directly relevant to membrane performance [1-3].

In this contribution, SSNMR applications to anion exchange membranes for water electrolysis will be presented, with particular focus on the interplay between polymer segmental dynamics under hydrated conditions and adsorbed water mobility. Variable-temperature ^{1}H time-domain NMR experiments were used to investigate polymer chain dynamics and determine an NMR-derived glass transition temperature under dry and hydrated conditions. In parallel, static ^{2}H NMR spectra of membranes equilibrated under controlled hydration with D_2O were analysed as a function of temperature to probe the mobility and dynamic heterogeneity of adsorbed water molecules, allowing different dynamic environments of confined water to be distinguished.

The combined ^{1}H and ^{2}H NMR approach provides a molecular picture of how hydration affects both the polymer matrix and confined water dynamics in AEMs, contributing to the understanding of structure-dynamics-property relationships in membranes for electrochemical energy applications.

Acknowledgments: PRIN PNRR 2022 "In MoTion-Influence of dynaMics on the adsorption and Transport properties in polymeric materials for membrane technologies" funded by the European Union - Next Generation EU is acknowledged for financial support.

References:
[1] B. Reif et al., *Nat. Rev. Methods Primers*, 1, (2021), 2
[2] A.R. Hughes et al., *Cryst. Eng. Comm.*, 23, (2021), 2491-2503
[3] K. Schmidt-Rohr et al., *Multidimensional Solid-State NMR and Polymers* Vol. 478 (Academic, 1994)

Origin of the linear heat-capacity term in Graphite-Based Nanomaterials

O.I. Kryvchikov[1,2*], A. Jeżowski[2], D. Szewczyk[2], M.S. Barabashko[1], O.A. Korolyuk[1]

[1] B. Verkin Institute for Low Temperature Physics and Engineering, NAS of Ukraine, Nauky Ave. 47, 61103 Kharkiv, Ukraine
[2] Institute of Low Temperature and Structure Research PAS, Okólna 2, 50-422 Wrocław, Poland

Low-temperature heat capacity is a sensitive probe of low-energy excitations in carbon materials, where dimensionality, disorder, and interlayer interactions strongly influence thermodynamic properties. In this work, we investigate the low-temperature specific heat of three graphite-derived nanomaterials: multi-walled carbon nanotubes (MWNTs)[1], exfoliated graphite (EG)[2], and graphene oxide (GO)[3]. These materials differ significantly in morphology, defect concentration, and structural ordering, providing an opportunity to identify the factors responsible for deviations from the conventional Debye model.

All studied materials exhibit a pronounced linear contribution to the heat capacity at low temperatures, in addition to the lattice term. The magnitude of this contribution depends strongly on the structural state of the material. In MWNTs, the linear term is associated with low-dimensional vibrational excitations characteristic of nanotube assemblies and may include a small electronic contribution from metallic nanotubes. In EG, it reflects the effects of weak interlayer coupling, structural anisotropy, and defects generated during the exfoliation process. The largest linear contribution is observed in GO, where a high concentration of structural defects and oxygen-containing functional groups gives rise to disorder-induced low-energy excitations, including localized vibrational states and two-level systems.

The comparative analysis demonstrates that the linear heat-capacity term is not a universal property of graphitic materials but is highly sensitive to their dimensionality, defect structure, and degree of disorder. The results indicate that both low-dimensional phonon modes and disorder-related excitations contribute to the low-temperature thermodynamic behavior of graphite-derived nanostructures. These findings highlight the usefulness of low-temperature calorimetry as a tool for probing the microscopic structure and low-energy dynamics of carbon materials beyond the framework of the Debye model.

References:
[1] M.S. Barabashko et al., *Carbon Trends*, 19, (2025), 100479
[2] A.I. Krivchikov et al., *J. Appl. Phys.*, 139 (2026), 144304
[3] A.I. Krivchikov et al., *Nanoscale Microscale Thermophys. Eng.*, 29, (2026), 219-233

Tiny movements, big change: when collective small displacements control flow and aging in soft matter

S.S. Napolitano[1]

[1] Laboratory of Polymer and Soft Matter Dynamics, Experimental Soft Matter and Thermal Physics (EST), Université libre de Bruxelles (ULB), Brussels 1050, Belgium

At thermodynamic equilibrium, the properties of a system remain constant in time. Most processes in nature, however, occur far from it, and the gradual relaxation of materials toward lower-energy states ultimately determines their lifetime, stability, and function. At the molecular level, equilibration kinetics are governed by molecular motion, establishing a direct link between equilibrium properties and nonequilibrium dynamics [1].

In liquids and soft materials, equilibration is commonly associated with structural (α-) relaxation, which underlies glass formation and slows dramatically upon cooling. Yet growing evidence shows that many relaxation processes follow a markedly weaker temperature dependence, decoupled from α-relaxation entirely. We attribute this behavior to the slow Arrhenius process (SAP) [2], the experimental signature of a distinct mode of molecular motion driven by collective small displacements (CSD): localized, coordinated motions of limited amplitude that do not require large-scale structural rearrangement [3].

Combining this mechanism with a statistical-mechanical description of intermolecular interactions yields a predictive framework that quantitatively links molecular-scale dynamics to macroscopic relaxation rates, from equilibrium measurements alone and without free parameters. The framework, validated across systems and lengthscales, predicts mechanisms like crystal growth kinetics in pharmaceutical and organic electronic compounds [4], molecular exchange times in biological membranes [5], and polymer adsorption kinetics on semiconductor surfaces [6]. A key and perhaps unexpected result is that physical aging in the glassy state and viscous flow at high temperature share the same thermal barrier, pointing to a common microscopic origin across the full temperature range and suggesting a unified picture of slow dynamics in soft and disordered matter.

References:
[1] L. Onsager, *Phys. Rev.*, 37, (1931), 405-426
[2] Z. Song et al., *Sci. Adv.*, 8, (2022), eabm7154; F. Caporaletti and S. Napolitano, *Phys. Chem. Chem. Phys.*, 26, (2024), 745; E. Thoms and S. Napolitano, *J. Chem. Phys.*, 159, (2023), 161103; E. Thoms et al., *J. Phys. Chem. Lett.*, 15, (2024), 4838; F. Caporaletti, H. Bock, and S. Napolitano, *J. Mol. Liq.*, 433, (2025), 127902
[3] R.P. White, S. Napolitano, and J.E.G. Lipson, *Phys. Rev. Lett.*, 134, (2025), 098203
[4] F. Caporaletti et al., *Mater. Hor.*, 13, (2026), 491-498
[5] K. Wang et al., *Small*, 22, (2026), e12844
[6] E. Thoms et al., *Phys. Rev. Lett.*, 132, (2024), 248101

Calorimetric studies on melting of rubbers under strain

H. Suzuki[1]

[1] Department of Chemistry, Kindai University, Higashiosaka, Osaka 577-8502, Japan

Rubbers consist of crosslinked polymer chains that are in a liquid-like state; that is, the randomly oriented polymer chains undergo thermal motion under the constraints imposed by crosslinkers. Upon cooling, rubbers can crystallize. In natural rubber, it is also known that crystallization can occur upon stretching. The former is referred to as thermally induced crystallization (TIC), and the latter as strain-induced crystallization (SIC). From a thermodynamic viewpoint, SIC can be interpreted as follows: the application of uniaxial force aligns the polymer chains, reducing their conformational entropy and thereby destabilizing the liquid state. However, experimental evaluations of changes in energy and entropy during stretching have been limited.

In this study, we investigated the effect of uniaxial strain on the melting behavior of rubber using a high-precision adiabatic calorimeter.[1] As a result, the melting signal of SIC was not clearly observed, whereas the melting temperature of TIC was found to shift slightly (by approximately 4 K) upon fourfold stretching. This small increase in melting temperature appears to be universal for rubbers, irrespective of the occurrence of SIC. The variation of entropy and internal energy upon stretching in the rubbery (liquid) state was also investigated by stress and elatsocaloric measurements, which revealed that the small increase in melting temperature is mainly due to the entropy reduction in the rubbery (liquid) state.

References:
[1] M. Umeda, T. Wakabayashi, T. Kamiyama, and H. Suzuki, *Polymer*, 254, (2022), 125105

Acceleration of the crystal growth across the liquid to glass transition

D. Sonaglioni[1,2], E. Tombari[2], S. Capaccioli[1,2,3]

[1] Dipartimento di Fisica, Università di Pisa, Pisa, Italy, danielesonaglioni@cnr.it
[2] Istituto per i Processi Chimico-Fisici del CNR (IPCF-CNR), Pisa, Italy, elpidio.tombari@cnr.it
[3] CISUP, Centro per l'Integrazione della Strumentazione dell'Università di Pisa, Pisa, Italy, simone.capaccioli@unipi.it

Isothermal crystallization is a highly debated topic in Soft Matter Physics. According to the Classical Nucleation Theory (CNT) [1], crystallization in the supercooled liquid state is affected by the diffusion coefficient. However, crystallization may arise in the glassy state as well, known as GC growth [2], a state of matter usually thought of as frozen. As noted by many authors, GC growth is characterized by an acceleration of the crystallization rates when crossing the glass transition temperature, showing an Arrhenius dependence from temperature, accompanied by a change in the morphology of the growing crystals [2]. At the state of the art, a final understanding of GC growth is still lacking.

In this study, we exploited the fast and fine control of sample temperature enabled by Fast Calorimetry, to investigate the crystallization kinetics of a highly crystallizable compound from the supercooled liquid and from the glassy states, unveiling the emergence of GC growth. To gain deeper understanding on GC growth, we tested the effect of the cooling rate for sample preparation in the glassy state and interpreted the obtained results in terms of out-of-equilibrium degree and the number of nuclei, employing an extended version of CNT.

The obtained results have shed light on novel aspects of GC growth, and the evidence gathered has allowed us to interpret this phenomenon as being driven by a fast local dynamics active in the bulk state and decoupled from structural relaxation below the glass transition temperature [3].

References:
[1] J.F. Loffler et al., *Appl. Phys. Lett.*, 77, (2000), 681-683
[2] Y. Sun et al., *J. Phys. Chem. B*, 112, (2008), 661-664
[3] D. Sonaglioni et al., *Phys. Rev. Mater.*, under revision

Probing structure and dynamics in functional porous materials by solid state NMR spectroscopy

F. Martini[1,2], E. Della Latta[1], F. Nardelli[1,2,3], S. Borsacchi[2,3], L. Calucci[2,3], M. Geppi[1,2]

[1] Department of Chemistry and Industrial Chemistry, University of Pisa, v. G. Moruzzi 13, 56124 Pisa, Italy, francesca.martini@unipi.it
[2] Center for Instrument Sharing of the University of Pisa (CISUP), 56124 Pisa, Italy
[3] Institute for the Chemistry of Organometallic Compounds, National Council of Research (ICCOM-CNR), v. G. Moruzzi 1, 56124 Pisa, Italy

Coordination polymers (CPs) are crystalline materials formed by metal ions or clusters interconnected by organic ligands through coordination bonds [1]. This broad class of functional materials includes metal–organic frameworks (MOFs), which are characterized by permanent porosity and high surface area. Owing to their tunable structures and adsorption properties, CPs are attracting growing interest for pressing environmental and biomedical applications, including gas capture, pollutant removal, and drug delivery. Understanding host–guest interactions and molecular dynamics is crucial for optimizing their performance.

This contribution highlights the role of solid-state NMR spectroscopy (ssNMR) in the characterization of functional CPs through selected case studies. Examples include Ce-based MOFs for CO_2 capture [2], 1D CPs for volatile organic compound (VOC) adsorption [3], and MOF-based drug delivery systems. By combining multinuclear high- and low-resolution ssNMR experiments with nuclear spin relaxation measurements at variable temperature, information on local structure, molecular mobility, and confinement effects can be obtained at the atomic scale. These studies demonstrate the capability of ssNMR to provide unique molecular-level information on host–guest interactions and dynamics in porous materials, providing valuable guidelines for the design of advanced porous materials for environmental and biomedical applications.

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References:
[1] S. Kitagawa et al., *Angew. Chem. Int. Ed.*, 43, (2004), 2334-2375
[2] F. Nardelli et al., *J. Phys. Chem. C*, 128, (2024), 16, 6887-6896
[3] E. Della Latta et al., *Chem. Eur. J.*, 31, (2025), e202501458

NMR and NQR of functional materials for environmental, energy, and optoelectronic technologies

E. Della Latta[1], A. Scarperi[1,2], G. Rossi[1], E. Carignani[2,3], F. Nardelli[1,3], F. Martini[1,3], S. Borsacchi[2,3], M. Geppi[1,3]

[1] Department of Chemistry and Industrial Chemistry, University of Pisa, v. G. Moruzzi 13, 56124 Pisa, Italy, marco.geppi@unipi.it
[2] Institute for the Chemistry of Organometallic Compounds, National Council of Research (ICCOM-CNR), v. G. Moruzzi 1, 56124 Pisa, Italy
[3] Center for Instrument Sharing of the University of Pisa (CISUP), 56124 Pisa, Italy

In this keynote lecture the potential of multi-nuclear solid state Nuclear Magnetic Resonance (ssNMR) and Nuclear Quadrupole Resonance (NQR) spectroscopies for the investigation of functional materials will be highlighted through the discussion of recent applications to different classes of materials, with particular emphasis on their molecular-level structural and dynamic properties.

Examples will include studies of: halide mixing and photo-induced segregation (Hoke effect) in mixed-halide perovskites by ^{207}Pb ssNMR and $^{79/81}$Br and ^{127}I NQR, including under illumination *in situ* experiments [1]; the dynamics of both the polymer matrix and carbon dioxide guest molecules in Polymers with Intrinsic Microporosity (PIMs) by ^{1}H, ^{19}F, ^{13}C, and ^{2}H ssNMR [2]; and the distribution of electronic charge carriers in Indium Tin Oxide (ITO) semiconductor nanocrystals by ^{119}Sn ssNMR [3].

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References:
[1] A. Scarperi et al., *J. Am. Chem. Soc.*, 147, (2025), 33799-33811
[2] E. Della Latta et al., *Macromolecules*, 57, (2024), 11152-11165
[3] A. Gabbani et al., *ACS Nano*, 18, (2024), 15139-15153

Electron correlation induced glasses in molecular compounds

Y. Nakazawa[1], H. Manabe[1], C.V. Arthurs[1], T. Nomoto[2], S. Yamashita[1], H. Akutsu[1], A. Krivchikov[3]

[1] Dept. of Chemistry, Graduate School of Science, the Univ. of Osaka, Japan
[2] RIKEN Center for Emergent Matter Science (CEMS), Japan
[3] B. Verkin Institute of Low Temperature Physics and Engineering, Kharkiv, Ukraine

A charge-glass (CG) state is considered as a metastable electronic state driven by electron correlations typically emerging in molecular charge transfer complexes. It appears in 1/4 filling electronic states of π–electron band with strong electron correlations and the electron-phonon interaction in typically in M_2X compounds, where M denotes electron doner/acceptor molecules and X is monovalent counter ions. In this electronic filling, owing to the inter-site Coulomb repulsion V which tends to form a charge ordering (CO) state with electron-rich or electron-poor sites. This is considered as a kind of Wigner lattice state of electrons with superlattice periodicity. However, if the molecular stacking in the electron donor/acceptor layer has a frustration factor, which disturbs formation of suitable charge ordering pattern, glass freezing of electron density manifest itself in low temperature region. BEDT-TTF (bis(ethylenedithio)tetrathiafulvalene) based charge-transfer salts with the θ–type donor arrangement is a typical material which shows such CO and CG states. We have developed a new apparatus to measure accurate heat capacity and thermal conductivity for tiny single crystal samples less than 100 μg of molecular compounds and performed detail and systematic thermodynamic studies of these materials.

In the case of θ–$(BEDT\text{-}TTF)_2CsZn(SCN)_4$ in which CG state is realized, the low temperature heat capacity has a hump-like structure in its C_pT^{-3} vs T plot, reminiscent of a boson peak of glassy materials. [1)] In addition, at around 100 K, which is the characteristic temperature range where charge glass is formed, we observed a slight structure in the temperature dependence of the heat capacity due to glass formation of charges.[2-3] We discuss peculiar dynamics of the glassy formation and characterize the character of charge glass transition based on the temperature and the frequency dependences of the AC heat capacity. We also discuss cooling rate dependence of θ–$(BEDT\text{-}TTF)_2RbZn(SCN)_4$ and investigate the difference of lattice state between the well-ordered CO state and the glassy state. The strong electron correlations and large charge-lattice coupling is considered as a new mechanism to induce disordered phonon structure in regular lattice in molecular crystals.

References:
[1] R. Yoshimoto et al. *Physica B*, 449, (2014), 19-24
[2] T. Nomoto and Y. Nakazawa et al., *J. Phys. Soc. Jpn*., 88, (2019), 073601
[3] T. Nomoto and Y. Nakazawa et al., *Phys. Rev. B*, 107, (2023), 124803

Scaling laws of electrical conductivity in conductive materials: length-scale and universality

A. Serghei[1]

[1] Université Claude Bernard Lyon1, Ingénierie des Matériaux Polymères, CNRS UMR 5223, 69622 Villeurbanne, France

The scaling laws governing the electrical and dielectric response of electronic and ion-conductive materials are discussed in the present contribution. A universal behavior is reported for both types of conductivity, intimately related to the length-scale of the charge transport phenomena. It will be shown that the characteristic frequencies defining the electrical and dielectric properties of ion-conductive materials show a universal behavior, irrespective of the chemical nature, temperature and ion concentration of the ionic materials. This universality, due to the length-scale of the molecular structure underlying the mechanism of ion-hoping and ion diffusion, has far-reaching consequences. Knowing the DC-conductivity of any ion-conducting material allows one to accurately determine its characteristic frequencies and reconstruct by that, in a broad frequency range, the whole spectral dependence of its electrical and dielectric properties.

For electronically conductive composite materials, a universal behavior is reported as well, linking the electromagnetic shielding effectiveness to the value of conductivity. For numerous experimental results, obtained in our laboratory or reported in the scientific literature, we show that, irrespective of the nature of the conductive material (carbon based or metallic) and of the nature of the polymer matrix, the correlation between the electromagnetic shielding effectiveness, electrical conductivity and sample thickness follows a universal behavior, all experimental points falling onto a single universal curve. This universal behavior is due to the huge gap between the length-scale of the electrical percolation phenomenon and the characteristic length-scale of the electromagnetic wave propagation. The universal relationship found in our study opens the perspective of a precise predictive determination of the electromagnetic interference shielding effectiveness of composite materials based solely on their electrical properties.

References:

[1] “Dielectric Properties of Ionic Liquids at Metal Interfaces: Electrode Polarization, Characteristic Frequencies, Scaling Laws”, by A. Serghei, M. Samet, G. Boiteux, A. Kallel in the book “Dielectric Properties of Ionic Liquids” ed. Marian Paluch, Springer (2016)

[2] C. Retailleau, J. Alaa Eddine, F. Ndagijimana, F. Haddad, B. Bayard, B. Sauviac, P. Alcouffe, M. Fumagalli, V. Bounor-Legaré, and A. Serghei, *Comp. Sci. Technol.*, 221, (2022), 109351

[3] H. Lecocq, N. Garois, O. Lhost, P.-F. Girard, P. Cassagnau, and A. Serghei, *Comp. Part B*, 189, (2020), 107866

Identifying molecular moieties incorporated in charge transport and their contribution to conductivity

A.M. Anton[1]

[1] Leibniz Institute of Surface Engineering (IOM), Permoserstr. 15, 04318 Leipzig, markus.anton@iom-leipzig.de

Broadband dielectric spectroscopy and Fourier-transform infrared (FTIR) spectroscopy are combined in order to study charge transport and the role of individual molecular moieties on the example of polymerized ionic liquids (polyILs). Dielectric spectroscopy probes the complex conductivity and dielectric relaxation over a broad frequency and temperature range, providing access to charge transport and collective relaxation processes. In contrast, FTIR spectroscopy yields site-specific information on sub-molecular vibrations and their evolution during thermal cycling. By combining both techniques, distinct sub-molecular moieties are identified that are correlated to charge transport, while other part of the same molecule remain largely decoupled from conductivity processes [1]. In addition, a benchmark polyIL exhibiting remarkably high DC conductivity is studied in detail. Notably, longer polymer chains show enhanced conductivity compared to shorter analogues despite higher glass transition temperature and thus slower segmental dynamics [2]. This polymer system forms an extended hydrogen-bond network, from which binding partners are identified and their role in charge transport is quantified. During thermal cycling, the density of hydrogen-bonded protons varies by a factor of 4, whereas the DC conductivity changes by orders of magnitude [3]. These results indicate that charge transport is predominated governed by hopping conduction assisted through glassy dynamics, with hydrogen bonding exerting at most a minor influence on charge transport. The presented combined spectroscopic approach provides a comprehensive framework to link molecular interactions, relaxation processes, and macroscopic transport.

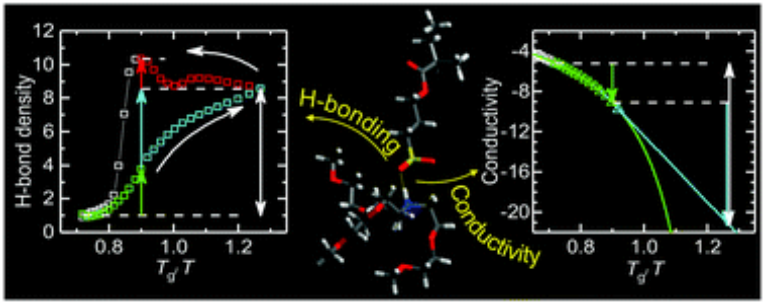

Figure 2. Variation of H-bond density and DC conductivity during temperature cycling [3].

References:
[1] F. Frenzel et al., *Soft Matter*, 15, (2019), 1605-1618
[2] F. Frenzel et al., *Macromolecules*, 55, (2017), 4022-4029
[3] A.M. Anton et al., *Soft Matter*, 612, (2023), 287-290

Chemically modified 2D materials: Unlocking new properties and functionalities

A. Forment-Aliaga[1], N.V. Vassylyeva[1], I. Brotons-Alcázar[1], B. Alba-Sangrós[1], M. Morant-Giner[1], D.A. Céspedes-Llanos[1], and E. Coronado[1]

[1] Instituto de Ciencia Molecular-Universitat de València. C/ Catedrático José Beltrán, 2, Paterna, Valencia, 46980 Spain, alicia.forment@uv.es

Two-dimensional materials (2Dms) are a family of nanomaterials consisting of ultrathin layers just a few atoms thick. Electron confinement in two dimensions, combined with their exceptionally high surface-to-volume ratio, gives rise to unique electronic, optical, and mechanical properties. New functionalities can be introduced through chemical modification with tailored molecular systems. In this context, we have functionalized 2D transition metal chalcogenides (TMCs) using coordination compounds, polyoxometalates, and chiral molecules. [1] Here, we present selected examples demonstrating how these modifications enable the incorporation of additional functionalities, enhancing the potential of these nanomaterials for energy, optoelectronic, and spintronic applications. We also discuss innovative strategies for the asymmetric functionalization of 2DMs, leading to the fabrication of Janus 2DMs. [2]

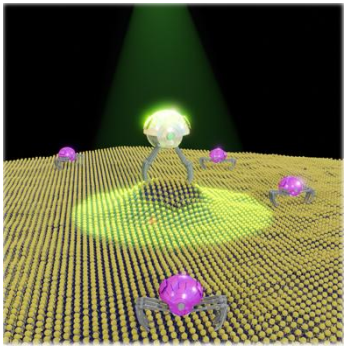

Figure 3. Artistic representation of the covalent functionalization of MoS_2 with spin-crossover nanoparticles during spin state transition process [1].

Comprehensive characterization of functionalized 2Dms remains challenging, as conventional techniques often lack the spatial resolution and sensitivity required to fully capture their surface properties. Scanning Probe Microscopy (SPM) partially overcomes these limitations, enabling nanoscale mapping of chemical, mechanical, and electronic properties with lateral resolution. Here, we present selected examples illustrating the power of SPM to prove mechanical and spin transport properties of functionalized 2Dms. [3]

References:

[1] R. Torres-Cavanillas et al., *Nat. Chem.*, 13, (2021), 1101-1110
[2] N. V. Vassilyeva, A. Forment-Aliaga, and E. Coronado, *Small*, 22, (2026), 2406599
[3] I. Brotons-Alcázar et al., *ACS Appl. Mater. Interfaces*, 16, (2024), 19711-19719

FLASH TALKS

16:45 **Monika Brzostowicz** (Kraków, Poland)

Structural, thermal, and vibrational properties of glycine–chloranilic acid – a new complex

16:50 **Juliusz Chojenka** (Kraków, Poland)

Low-temperature semiconductor-to-insulator transition in the Ti/TiO2/Fe system

16:55 **Mariya Mathew** (Chorzów, Poland)

Balancing thermal robustness and physical stability: co-amorphous CBD-MEL systems under forced stress conditions

17:00 **Svitlana Pastukh** (Kraków, Poland)

Quantifying anharmonic effects on Raman spectra and thermal conductivity in β-$FeSi_2$ from first principles

17:05 **Abinaya Rengarajan** (Kraków, Poland)

Controlling ion migration in argyrodites for stable thermoelectric devices

17:10 **Wojciech Sas** (Kraków, Poland)

Pressure-induced spin-crossover in a 2D Hofmann clathrate studied by X-ray absorption spectroscopy

17:15 **Sagarika Sharma** (Kraków, Poland)

Thermal stability limits of Cu-based argyrodites: phase evolution and degradation in $Cu_8SiS_3Se_3$

17:20 **Michał Stekiel** (Munich, Germany)

Magnetic excitation spectrum and hierarchy of magnetic interactions in $ErFeO_3$

Structural, thermal, and vibrational properties of glycine–chloranilic acid – a new complex

M. Brzostowicz[1], J. Hetmańczyk[2], Ł. Hetmańczyk[2]

[1] Jagiellonian University, Doctoral School of Exact and Natural Sciences, Prof. St. Łojasiewicza St 11, PL30348, Cracow, Poland, Jagiellonian University in Cracow, Faculty of Chemistry, Gronostajowa 2, 30-387 Cracow, Poland, monika.brzostowicz@uj.edu.pl
[2] Jagiellonian University in Cracow, Faculty of Chemistry, Gronostajowa 2, 30-387 Cracow, Poland

Chloranilic acid (CLA) is a proton donor that simultaneously exhibits electron affinity due to its quinoid structure, making it a suitable candidate for studies of hydrogen bonding and charge-transfer (CT) complexes, as well as their stability. Moreover, the presence of two equivalent –OH groups enable participation in supramolecular interactions [1]. It is well established that combining simple molecular systems, such as amino acids with organic compounds, can lead to the emergence of new physicochemical properties not observed in the individual components [2].

In this work, the glycine–chloranilic acid complex was investigated. At room temperature, the compound crystallizes in the triclinic system (space group P–1) and is isostructural with the N,N-dimethylglycine–chloranilic acid complex [1]. The polymorphic behavior and thermal stability of the system over a wide temperature range were examined using differential scanning calorimetry (DSC) and thermogravimetric (TG) analysis. DSC measurements revealed a reversible phase transition at 271 K upon heating and 249 K upon cooling. The observed thermal hysteresis of approximately 22 K, together with the sharp heat flow anomaly, indicates a first-order phase transition.

The entropy changes associated with the transition suggest significant configurational disorder in the high-temperature phase, characteristic of order–disorder (ODIC) crystals [3]. X-ray diffraction and NMR spectroscopy indicate the presence of protonated glycine species alongside deprotonated chloranilic acid dimers stabilized by strong O–H···O hydrogen bonds. The dynamic properties of the complex were investigated using temperature-dependent mid- and far-infrared spectroscopy (MIR and FIR), allowing the determination of activation energies for reorientational motions. Experimental IR spectra were compared with theoretical spectra calculated using density functional theory (DFT) under periodic boundary conditions (Quantum Espresso), showing good qualitative agreement. DFT calculations for isolated molecular models further supported the interpretation of vibrational features. Hirshfeld surface analysis was also performed to characterize intermolecular interactions and quantify key contacts within the crystal structure.

These findings provide comprehensive insight into the interplay between proton transfer, hydrogen bonding, and lattice dynamics, offering a deeper understanding of phase transitions in molecular charge-transfer systems.

References:
[1] J. Hetmańczyk, Ł. Hetmańczyk, W. Schilf, *Materials*, 14(12), (2021), 3292
[2] M. Zaman, M. Tomura, Y. Yamashita, *J. Org. Chem.*, 66(18), (2001), 5987-5995
[3] Dynamics of Solids and Liquids by Neutron Scattering, *Topics in Current Physics*, 3, (1977), S. W. Lovesey and T. Springer (eds.)

Low-temperature semiconductor-to-insulator transition in the Ti/TiO_2/Fe system

J.C. Chojenka[1], A. Zarzycki[1], A. Vibhakar[2], A. Bombardi[2], M. Krupiński[1]

[1] Institute of Nuclear Physics Polish Academy of Sciences, PL-31342 Krakow, Poland, juliusz.chojenka@ifj.edu.pl
[2] Diamond Light Source Ltd, Harwell Science and Innovation Campus, Didcot, Oxfordshire, UK.

Titanium dioxide is a wide-band-gap semiconductor with promising properties for applications in energy storage, hydrogen generation, and photocatalysis. Moreover, TiO_2-based resistive switching devices offer significant potential for developing novel neural networks as artificial synapses. This is possible because TiO_2 exhibits a resistive switching effect, which occurs when it is sandwiched between two metallic electrodes. However, stoichiometric titanium dioxide can be readily reduced through chemical reactions at the interface with certain metals, such as W or Ni. This interaction at the metal–oxide interface facilitates the formation of a high concentration of oxygen vacancies, which in turn leads to the formation of TiO_2 suboxides.

To demonstrate the influence of titanium suboxides on the electrical properties of the Ti/TiO_2/Fe system, we present results of our investigation of temperature-dependent resistance, correlated with the system's crystal structure. The resistance of the heterojunction exhibits three regimes: a single Schottky junction at high temperatures, a double Schottky junction at intermediate temperatures, and insulating behavior at low temperatures. The final regime corresponds to a transition to an insulating state at low temperatures, which is related to the reduction of TiO_2.

Our investigation revealed the presence of Ti_3O_5 and Ti_4O_7 phases. We suggest that the formation of these phases results from the reduction of TiO_2 at the interface with the iron layer, as well as enhanced internal stress at low temperatures. The formation of an insulating layer at the interface is responsible for the observed semiconductor-to-insulator transition.

Balancing thermal robustness and physical stability: co-amorphous CBD–MEL systems under forced stress conditions

M. Mathew[1], J. Knapik-Kowalczuk[1], M. Paluch[1]

[1] Institute of Physics, Faculty of Science and Technology, SMCEBI, University of Silesia in Katowice, 75 Pułku Piechoty 1a, 41-500 Chorzów, Poland, mariya.mathew@us.edu.pl

Cannabidiol (CBD) is a pharmacologically active compound with broad therapeutic potential; however, its clinical application is significantly limited by poor aqueous solubility and low oral bioavailability. Amorphization is a promising strategy to enhance dissolution and apparent solubility, yet it is often constrained by poor physical stability and a strong tendency toward recrystallization. Although amorphous CBD shows relative stability under ambient conditions, it remains highly susceptible to pressure-induced recrystallization, underscoring the need for effective stabilization strategies.

A co-amorphous system combining CBD and melatonin (MEL) is explored as an approach to improve physical stability. MEL, a bioactive molecule with antioxidant and chronobiotic properties, is selected as a co-former based on its demonstrated potential in co-amorphous systems and its complementary pharmacological profile. Accordingly, co-amorphous CBD–MEL mixtures were prepared and characterized using thermogravimetric analysis (TGA), differential scanning calorimetry (DSC), and broadband dielectric spectroscopy (BDS). The eutectic composition was identified at CBD + 20% MEL based on experimental results supported by Schroeder–van Laar predictions. This composition exhibited the most favorable thermal properties and was therefore selected for high-pressure dielectric experiments.

The dielectric measurements performed under ambient and high-pressure conditions at 298 K demonstrate that the incorporation of 20% MEL significantly suppresses recrystallization and enhances the physical stability of amorphous CBD. These findings highlight MEL as an effective stabilizing co-former, supporting the development of robust co-amorphous formulations with improved pharmaceutical potential.

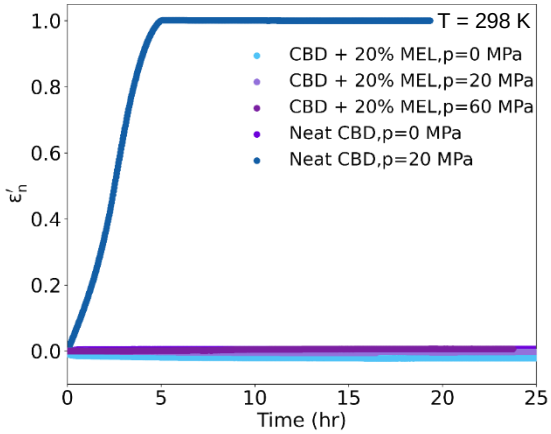

Figure 4. Crystallization Kinetics of Neat CBD and CBD + 20% MEL under ambient and elevated pressure at room temperature.

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References:

[1] M. Mathew, J. Knapik-Kowalczuk, M. Dulski, and M. Paluch, *Pharmaceutics*, 17, (2025), 358

Quantifying anharmonic effects on Raman spectra and thermal conductivity in β-$FeSi_2$ from first principles

S. Pastukh[1] and P. Piekarz[1]

[1] The Henryk Niewodniczański Institute of Nuclear Physics Polish Academy of Sciences ul. Radzikowskiego 152 31-342 Kraków, Poland, svitlana.pastukh@ifj.edu.pl

Iron silicides are promising materials for optoelectronic and thermoelectric applications [1], yet their thermal transport properties and the role of anharmonic effects remain not fully understood. In this work, we present a comprehensive ab initio study of lattice dynamics and phonon-mediated heat transport in the orthorhombic semiconductor β-$FeSi_2$.

Anharmonic effects are analyzed using both self-consistent phonon (SCPH) theory [2] and perturbation theory [3]. While SCPH yields only small renormalization of phonon frequencies, perturbative anharmonicity has a strong impact on phonon linewidths and selected optical modes. By combining Raman tensors with anharmonic phonon line shapes, we reproduce the temperature-dependent Raman spectra and resolve discrepancies with experimental linewidths.

Phonon lifetimes and group velocities are analyzed as functions of frequency, and the lattice thermal conductivity is evaluated over a broad range of temperatures and crystallite sizes. The results reveal weak anisotropy associated with the orthorhombic crystal structure and demonstrate that the third order anharmonic contributions play the dominant role in the thermal transport. The calculated thermal conductivity shows a good agreement with available experimental data, providing a consistent and validated description of heat transport in β-$FeSi_2$.

References:
[1] M.C. Bost, J.E. Mahan, *J. Appl. Phys*., 64, (1988), 2034-2037
[2] T. Tadano, S. Tsuneyuki, *Phys. Rev. B*, 92, (2015), 054301
[3] T. Tadano, S. Tsuneyuki, *J. Phys. Soc. Jap*., 87, (2018), 041015

Controlling ion migration in argyrodites for stable thermoelectric devices

A. Rengarajan[1], M. Pindel[1], S. Sharma[1], O. Cherniushok[1], K. Wojciechowski[1]

[1] Thermoelectric Research Laboratory, Department of Inorganic Chemistry, Faculty of Materials Science and Ceramics, AGH University of Krakow, Mickiewicza Ave. 30, 30-059 Krakow, Poland, abinaya@agh.edu.pl

Controlling ion migration in Cu- or Ag-based argyrodites has emerged as a critical strategy for optimizing their thermoelectric performance, particularly due to the strong coupling between ionic transport and electronic conduction. Though tuning compositional disorder, lattice polarizability, and Cu-site occupancy can modulate the migration pathways and activation energy of mobile Cu ions. While material-level tuning is well explored, device-level implementation remains underdeveloped. In this work, we present a systematic design approach to engineer-controlled Cu-ion migration in argyrodites, aiming to enhance device stability and efficiency. The quantification of critical voltage (V_c) where ionic conductance exceeds baseline electronic leakage by >10% [1] has been performed in home-made four-probe set-up. The increased V_c is noticed for prepared argyrodites relative to binary analogues, explicitly arising from engineered defect landscapes that hinder Cu-ion migration. This enables suppression of detrimental ion drift under an applied electric field while preserving the intrinsically low lattice thermal conductivity characteristic of argyrodites [2]. A comprehensive understanding of ionic conductivity in argyrodites provides critical insights into the design and optimization of stable thermoelectric devices.

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References:

[1] K.A. Borup et al., *Energy Environ. Sci.*, 8, (2015), 423-435
[2] P. Taras et al., *Adv. Funct. Mater.*, 34, (2025), 2502163

Pressure-induced spin-crossover in a 2D Hofmann clathrate studied by X-ray absorption spectroscopy

W. Sas[1], P. Konieczny[1], A. Pacanowska[1], A. Rogalev[2], F. Wilhelm[2], A. Maximenko[3], G. Gazdowicz[3], M. Fitta[1]

[1] Institute of Nuclear Physics Polish Academy of Sciences, Radzikowskiego 152, 31-342 Kraków, Poland, wojciech.sas@ifj.edu.pl

[2] ESRF – The European Synchrotron Radiation Facility, CS 40220, 38043 Grenoble, Cedex 9, France

[3] SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, ul. Czerwone Maki 98, 30-392 Kraków, Poland

Spin-crossover (SCO) compounds are prominent candidates in multifunctional materials because of their bistable nature and porous structures. Within this class, Hofmann clathrates – coordination polymers built from 2D $[M^{II}(CN)_4]^{2-}$ layers linked by organic ligands – stand out for their robustness. In contrast to many molecular systems, they typically exhibit isostructural transitions, where the framework remains preserved while bond lengths vary, enabling excellent cycling stability.

In this work, we investigate the pressure-induced SCO behavior in a 2D iron-nickel Hofmann clathrate: {[Fe(pyridazine)$_2$Ni(CN)$_4$]}, Fe(pdz)Ni, by X-ray absorption spectroscopy (XAS) using a diamond anvil cell (DAC). In particular, we study the evolution of the spin-state during the application of pressure within the range 0-1.04 GPa, and compare it to the temperature-driven spin transition at ambient pressure. The results show that Hofmann clathrates are promising candidates for sensitive pressure-temperature sensors.

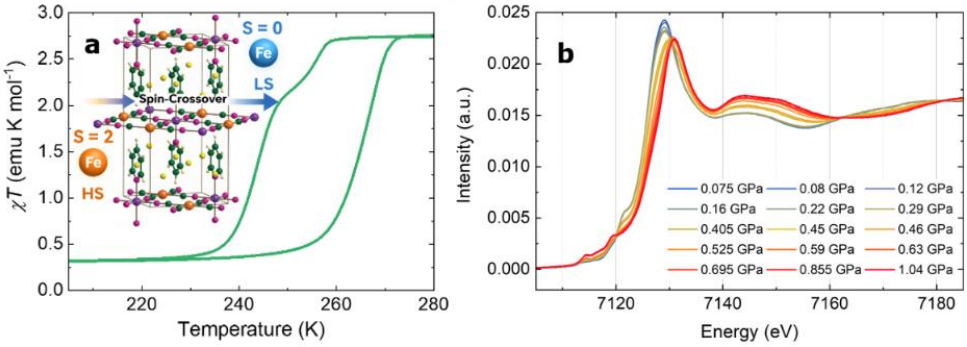

Figure 5. Magnetic susceptibility vs. temperature and crystal structure of Fe(pdz)Ni (a). Pressure-induced Fe K-edge XAS spectra of Fe(pdz)Ni (b).

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Thermal stability limits of Cu-based argyrodites: phase evolution and degradation in $Cu_8SiS_3Se_3$

S. Sharma[1], O. Cherniushok[1], T. Parashchuk[1], K. Pielichowska[2], K.T. Wojciechowski[1]

[1] Thermoelectric Research Laboratory, Department of Inorganic Chemistry, Faculty of Materials Science and Ceramics, AGH University of Krakow, 30-059 Krakow, Poland, ssharma@agh.edu.pl
[2] Department of Glass Technology and Amorphous Coatings, Faculty of Materials Science and Ceramics, AGH University of Krakow, Al. Mickiewicza 30, 30-059 Krakow, Poland

Cu-based argyrodites have attracted increasing attention as thermoelectric materials due to their intrinsically low thermal conductivity and promising electrical transport properties. However, their operational reliability is critically limited by insufficiently understood thermal stability, particularly under realistic environmental conditions. Here, we address this gap by introducing a quantitative framework for evaluating temperature-dependent stability and by establishing the operational limits of $Cu_8SiS_3Se_3$. We investigate phase stability, degradation pathways, and transport reversibility of $Cu_8SiS_3Se_3$ up to 873 K under inert (argon) and oxidative (air) conditions. High-temperature X-ray diffraction and thermogravimetric analysis are combined with cyclic transport measurements up to 773 K to directly assess structural and functional stability. To resolve degradation mechanisms, prolonged annealing at 873 K for 48 h is performed in vacuum and air, followed by cross-sectional SEM analysis to identify compositional gradients and volatile-element loss. Centre of this work, we introduce the Temperature Reversibility Index (TRI), a metric that quantifies the reversibility of transport properties during thermal cycling. We demonstrate that $Cu_8SiS_3Se_3$ maintains structural stability and reproducible transport properties only up to 473 K. Above this threshold, rapid degradation occurs. Under inert conditions, phase decomposition leads to $Cu_2(S,Se)$ and $Cu_2Si(S,Se)_3$, while exposure to air further accelerates degradation through oxidation, forming $CuSO_4$, Cu_2SO_5, and SiO_2. In both environments, selenium evaporation is the primary cause for degradation. TRI analysis provides a direct, quantitative measure of the collapse of transport reversibility and clearly shows the material's operational stability window. These results establish 473 K as the practical upper limit for reliable operation of $Cu_8SiS_3Se_3$ and identify the coupled effects of phase instability, oxidation, and volatile-element loss as the governing degradation mechanisms. More broadly, the TRI framework offers a generalizable tool for assessing stability limits in thermoelectric materials and enables more rational design of Cu-based argyrodites with improved thermal durability.

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References:
[1] T. Parashchuk, O. Cherniushok, B. Wiendłocha, J. Toboła, R. Cardoso-Gil, G.J. Snyder, Y. Grin, and K.T. Wojciechowski, *Adv. Funct. Mater.*, 35, (2025), 202502163

Magnetic excitation spectrum and hierarchy of magnetic interactions in $ErFeO_3$

D.R. Bhosale[1], P. Fabrykiewicz[1,2], D. Adroja[3,4], M. Meven[1,2], A. Schneidewind[1], M. Stekiel[1]

[1] Jülich Centre for Neutron Science at Heinz Maier-Leibnitz Zentrum, Forschungszentrum Jülich GmbH, Lichtenbergstraße 1, D-85747 Garching, Germany, m.stekiel@fz-juelich.de
[2] Institute of Crystallography, RWTH Aachen University, Jägerstraße 17–19, D-52066 Aachen, Germany
[3] ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, OX11 0QX, United Kingdom
[4] Highly Correlated Matter Research Group, Physics Department, University of Johannesburg, P.O. Box 524, Auckland Park 2006, South Africa

Rare-earth orthoferrites, $RFeO_3$ where R is a magnetic rare-earth ion, host two magnetic sublattices each governed by distinct energy scales, with the inter-sublattice coupling constituting a third, weaker scale. In particular, erbium orthoferrite with J=15/2 hosts Kramers degenerated 4f electron states, susceptible to perturbations [1] and giving rise to correlated magnetic effects, such as spin reorientation and spin switching [2].

We present a comprehensive investigation of the magnetic interactions in $ErFeO_3$, based on inelastic neutron scattering, in particular, neutron time-of-flight spectroscopy. Our measurements reveal a characteristic hierarchy of excitation energies in orthoferrites as well as the underlying hierarchy of magnetic interaction strengths. We characterize spin waves of the iron sublattice, crystal field (CEF) excitations of Er ions, splitting of the CEF levels, and spin-orbit coupling within iron sublattice, which together span the energy range from 100 to 0.1 meV [3].

Furthermore, we reveal the dispersive character of crystal field excitations of erbium, arising from Er-Er exchange coupling, and demonstrate the crucial role of dipolar interactions in the ground state splitting.

We present two theoretical frameworks: linear spin wave theory for spin waves and the Stevens formalism for CEF excitations, which are individually able to model the observed spectra, but cannot be straightforwardly unified. $ErFeO_3$ thus emerges as a vivid realization of multipolar magnetism, where spin and orbital degrees of freedom are deeply entangled. The observed hierarchy of interactions, and the limitations of existing theoretical frameworks, are likely universal features of the rare-earth orthoferrite family.

References:
[1] D.L. Wood et al., *Physical Review*, 185, (1969), 689-695
[2] I. Fita et al., *Phys. Rev. B*, 105, (2022), 094424
[3] D.R. Bhosale et al., *arXiv* 2604.27857, (2026)

Landscape of ordered phases in a localized-fermion system with on-site and intersite interactions on a triangular lattice

K.J. Kapcia[1], L. Regeciova[2], and J. Barański[3]

[1] Institute of Spintronics and Quantum Information, Faculty of Physics and Astronomy, Adam Mickiewicz University in Poznań, ul. Uniwersytetu Poznańskiego 2, 61614Poznań, Poland, konrad.kapcia@amu.edu.pl
[2] Institute of Experimental Physics, Slovak Academy of Sciences, Watsonova 47, 040 01Košice, Slovakia
[3] Department of General Education, Polish Air Force University, ul. Dywizjonu 303 nr 35, 08521 Deblin, Poland

A generalized fermionic lattice gas model in the form of the extended Hubbard model with intersite Ising-like interactions (between nearest neighbors, both antiferromagnetic and ferromagnetic) at the atomic limit on the triangular lattice is studied [1-5]. The Hamiltonian of the system consists of the following terms: nearest-neighbor Ising-like magnetic J interactions and onsite Coulomb U interactions. The model is investigated for both signs of J, arbitrary U interaction, and arbitrary chemical potential μ (or, equivalently, arbitrary particle concentration n) using two complementary methods: (i) Monte Carlo simulations in the grand canonical ensemble [1,3] and (ii) the variational method within the mean-field decoupling of the intersite term and exact treatment of the onsite interaction [2,3]. Both methods yield the exact ground-state phase diagram as a function of μ [1,2]. For antiferromagnetic coupling, a nontrivial ordered phase with coexistence of metamagnetic and charge ordering is found. The finite-temperature phase diagram is complex, with phase transitions between the ordered and nonordered phases being of first as well as second order (i.e., discontinuous and continuous, respectively), depending on the model parameters. The results are contrasted with the findings for the two-dimensional square lattice [3].

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References:

[1] L. Regeciová, K.J. Kapcia, *Phys. Rev. E*, 111, (2025), 064132
[2] K.J. Kapcia, J. Barański, *J. Magn. Magn. Mater.*, 591, (2024), 171702
[3] K.J. Kapcia, S. Murawski, W. Kłobus, and S. Robaszkiewicz, *Physica A*, 437, (2015), 218-234

Generalized Landau–de Gennes theory of polar and modulated nematic phases

P. Karbowniczek[1], L. Longa[2], Sz. Drzazga[3], A. Chrzanowska[4]

[1] Faculty of Materials Engineering and Physics, Cracow University of Technology, ul. Podchorążych 1, 30-084, Kraków, Poland
[2] Institute of Theoretical Physics and Mark Kac Center for Complex Systems Research, Jagiellonian University, ul. Łojasiewicza 11, 30-348 Kraków, Poland
[3] Institute of Theoretical Physics, Jagiellonian University, ul. Łojasiewicza 11, 30-348 Kraków, Poland
[4] Faculty of Materials Engineering and Physics, Cracow University of Technology, ul. Podchorążych 1, 30-084, Kraków, Poland

The understanding of self-organization in recently discovered nematic phases is at the forefront of soft-matter research worldwide [1, 2, 3, 4]. Several of these phases can develop local or long-range ferroelectric order, sometimes accompanied by structural chirality even though the constituent molecules are chemically achiral. Representative examples include the ferroelectric nematic phase NF and the heliconical ferroelectric nematic NTB,F. Closely related modulated nematic phases, such as the twist–bend nematic NTB and the splay–bend nematic NSB, provide a broader context for understanding the emergence of spontaneous orientational modulation and polar order.

Here we analyze polar and modulated nematics within a generalized Landau–de Gennes framework in which the alignment tensor field Q is coupled to a polarization field P through bulk polar terms and the lowest-order flexopolarization coupling [5]. To identify globally stable structures, we introduce a helicity-mode expansion of both Q and P and perform global numerical minimization within a class of one-dimensional periodic structures. We show that the polar sector of this theory, which has received little attention to date, stabilizes not only the experimentally observed ferroelectric and heliconical nematic phases, but also additional polar and modulated nematic structures that have not yet been observed experimentally. The resulting phase diagrams delineate the stability regions of isotropic, uniform nematic, polar, and modulated phases, revealing the interplay between bulk polarity, flexopolarization, and orientational self-organization.

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References:
[1] X. Chen et al., *Proc. Natl. Acad. Sci. U.S.A.*, 117, (2020), 14021
[2] J. Karcz et al., *Science*, 384, (2024), 1096
[3] S. Ghosh et al., *Matter*, 9, (2026), 102563
[4] L. Longa and W. Tomczyk, *J. Phys. Chem. C*, 124, (2020), 22761
[5] L. Longa and H.-R. Trebin, *Phys. Rev. A*, 42, (1990), 3453

Correlating experimental and DFT electronic structures of organic dopants for OLED materials

Z. Tokárová[1]

[1] Institute of Chemistry and Environmental Sciences, Faculty of Natural Sciences, University of Ss. Cyril and Methodius in Trnava, Nám. J. Herdu 2, 917 01 Trnava, Slovakia, zita.tokarova@ucm.sk

In the context of organic electronics, condensed matter refers to molecular and solid-state systems in which intermolecular interactions govern charge transport, energy transfer, and electronic structure. Nearly half a century after the emergence of organic electronics [1], optoelectronic devices continue to attract considerable scientific interest. Alongside established technologies such as OFETs and OPVs, OLEDs have regained significant attention due to the possibility of tuning their emission properties through the incorporation of molecular dopants.

DFT calculations performed at the TPSSH/6-31G(d) and B3LYP/6-31G(d,p) levels supported experimental findings obtained from cyclic voltammetry (CV) and energy-resolved electronic impedance spectroscopy (ER-EIS) for a series of low-molecular-weight organic compounds (**1b,c**; **2**; **3a,b**; **4b** and **5b**) synthesized and employed as dopants (**4b**; **5b**) in OLED devices exhibiting unusual yellow-green emission [2]. This study demonstrates the value of a combined experimental–theoretical approach for understanding the optoelectronic properties of organic condensed matter systems.

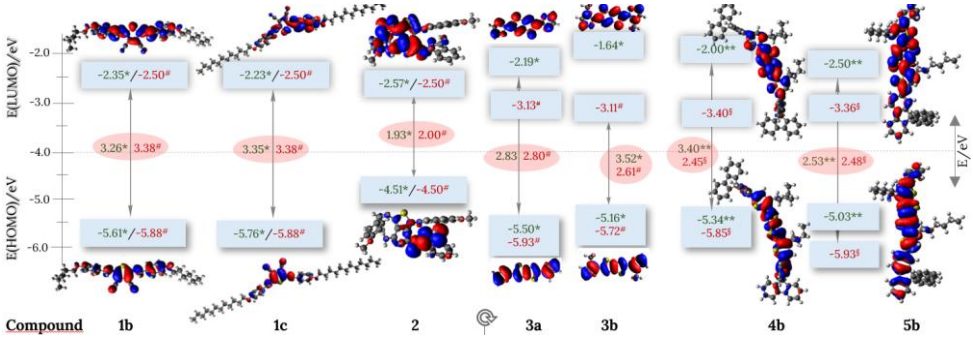

*Figure 6. Experimental (ER-EIS, §CV) vs. DFT (*B3LYP/6-31G(d,p), TPSSH/6-31G(d)) electronic energy levels for real organic dopants (**1b,c**; **2**; **3a,b**; **4b** and **5b**).*

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References:

[1] G. Xu, Y. Yang, Q. Chen, S.-Y.Xie, and Q. Zhang, *Adv.Funct. Mat.*, 36, (2026), e28875
[2] A. Eckstein-Andicsová, Z. Tokárová, E. Kozma, R. Balogh, A. Vykydalová, W. Mróz, K. Tokár, *New J. Chem.*, 47, (2023), 11165

Research on Bergman-type quasicrystals: disorder and stability

R. Strzałka[1], I. Bugański[1], J. Wolny[1]

[1] AGH University of Krakow, Faculty of Physics and Applied Computer Science, Mickiewicza 30, 30-059 Krakow, Poland

This presentation reviews our recent investigations into Bergman-type icosahedral quasicrystals within Zn-Mg-based systems containing transition metals or rare-earth elements. Our research employs a multi-method approach to resolve long-standing questions regarding the atomic structure, stability, and physical properties of these complex materials [1-3].

The structural part of our work combines single-crystal X-ray diffraction with advanced 3D modeling based on Ammann-Kramer-Neri tiling. By applying charge-flipping methods to reconstruct electron density maps, we have visualized positional disorder and identified a clear correlation: the degree of structural disorder decreases as the rare-earth element becomes heavier [4]. These experimental findings are supported by Density Functional Theory (DFT) calculations, which suggest that phase stability is driven by sp-d orbital hybridization rather than simple electronic concentration [5]. Finally, we discuss the synthesis and characterization of new Li-doped samples, which exhibit unique grain morphologies and offer fresh opportunities to study long-range magnetic ordering in quasicrystalline lattice [6].

References:
[1] I. Bugański, J. Wolny, and H. Takakura, *Acta Cryst. A*, 76, (2020), 180-196
[2] I. Bugański, R. Strzałka, and J. Wolny, *Acta Cryst. B*, 80, (2024), 84-93
[3] I. Buganski et al., *Acta Cryst. B*, 82, (2026), 175-185
[4] R. Strzałka et al., in prep.
[5] I. Bugański, R. Strzałka, and J. Wolny, *Isr. J. Chem.*, 64, (2024), e202300139
[6] I. Buganski et al., *Acta Cryst. A*, 82, (2026), S205327332501099X

Institute Laue-Langevin – instrument and infrastructure upgrades, the science strategy and new research opportunities for Poland

M. Johnson[1]
[1] Institut Laue Langevin, Grenoble, France, johnson@ill.eu

The comprehensive Endurance upgrade programme was completed in 2024. With a budget of 50+ M€, about 30 projects have been delivered, including neutron guide systems, new and upgraded instruments, sample environment and data and software services. More intense neutron beams combined with more efficient detector systems provide major new capability for measuring ever smaller samples, including in extreme sample environments, and weaker signals. In addition, significantly shorter measuring times facilitate parametric studies and increase throughput and, therefore, overall capacity. Thus the upgrade programme as a whole, supported by ongoing and new projects, ensures that research capability at the ILL will continue to be world leading for the next decade, offering new opportunities for cutting-edge science. In this context, the ILL has elaborated a science strategy to optimise the use of its state-of-the-art scientific infrastructure over the next decade and enhance the delivery of societal impact with neutrons.

The Endurance programme, ongoing and new projects, and the science strategy will be presented, including recent science highlights, and set in the context of future reactor operation to 2033 and beyond...

Solid-state study of a new venlafaxine and catechol cocrystal

G.P. Costa[1], G. Isquibola[2], J.G. dos Santos[1], P.O. Ferreira[3], F.F. Ferreira[3], M. Jamrógiewicz[4], F.J. Caires[1]

[1] School of Sciences, São Paulo State University, Bauru, 17033-360, SP, Brazil, gp.costa@unesp.br
[2] Institute of Chemistry, São Paulo State University, Araraquara, 14800-900, SP, Brazil
[3] LCCEM / CCNH, Federal University of ABC, Santo Andre, 09280-560, SP, Brazil
[4] Faculty of Pharmacy, Medical University of Gdańsk, Gdańsk, 80-416, Poland

This work reports the third cocrystal of venlafaxine, expanding the limited database of multicomponent solid forms of this clinically important antidepressant [1]. A systematic cocrystal screening was conducted using a mechanochemical method and catechol as coformer. The structure of the novel cocrystal was successfully solved from PXRD data, providing detailed insights into its crystal lattice, revealing a cocrystal in 1:2 stoichiometry. Hirshfeld surface analysis was employed to characterize the distribution and nature of intermolecular interactions within the cocrystal [2]. A binary phase diagram of the system showed the formation of one cocrystal and two eutectic mixtures at different stoichiometric ratios. All solid forms were further characterized using PXRD and IR spectroscopy, confirming their distinct structural and chemical features. Solubility studies showed that the cocrystal exhibited the highest solubility in comparison to the eutectic mixtures and drug, while the eutectics also enhanced solubility relative to the drug. These results indicate that the drug concentration in solution is primarily governed by the solubility of the cocrystal phase, while the eutectic systems contribute additional modulation through their less organized crystalline arrangements. The identification of a novel (1:2) venlafaxine-catechol cocrystal, alongside the characterization of eutectic mixtures, highlights the relevance of cocrystallization strategies for improving the bioavailability, physical stability, and potential therapeutic performance of poorly water-soluble drugs. These findings provide a framework for the rational design of multicomponent solid forms, with implications for future pharmaceutical development and optimization of drug formulations.

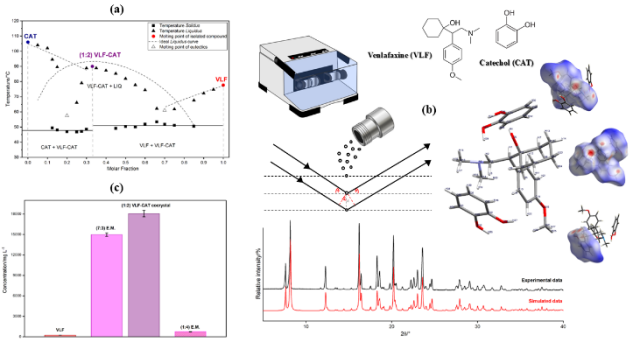

Figure 7. (a) Binary phase diagram, (b) diffractometric analysis, structural determination, Hirshfeld surface mapping, and (c) solubility profile of (1:2) VLF-CAT cocrystal.

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References:

[1] A.J. Gelenberg, R.B. Lydiard, R.L. Rudolph, L. Aguiar, J.T. Haskins, and E. Salinas, *JAMA – J. Am. Med. Assoc.*, 283, (2000), 3082-3088

[2] H. Yu, Y. Zhang, C. Xing, Y. Wang, H. Zhang, N. Gong, Y. Lu, and G. Du, *ACS Omega*, 6, (2021), 13895-13903

Study of imperfect structure in materials by Electron Diffraction

C.-W. Tai[1], S.F. Feng[1], B. Jeriga[1], A. Neagu[1]

[1] Department of Chemistry Stockholm University, Stockholm Sweden, cheuk-wai.tai@su.se

Functional materials are not necessary to be crystalline or defect-free. Crystallinity or defects are often considered to be key parameters, which can strongly influence the material properties. Transmission electron microscopy (TEM) is recognized as one of the essential characterization tools for materials research. TEM is particularly useful to examine the local features, deviated from the mean crystal structure and chemistry. Structural refinement helps to understand the structure-property relationship. However, the typical presentation – unit cell may not be able to describe precisely the local variations. Diffuse scattering, given by deviation of unit cell, can be intense features in an electron diffraction (ED) pattern, e.g. Figure 1 (left). If the structural disordering increase, the diffuse scattering can lose the distinct features in ED patterns but appears as diffuse background. Those are not related to Bragg diffraction. However, it is well-known that the features under the Bragg's peaks can be used to obtain pair-distribution function (PDF). In this presentation, PDF obtained in a TEM [1] and its applications to analysis several functional materials [2,3] having local structures, which cannot be examined by typical structural refinement, are discussed.

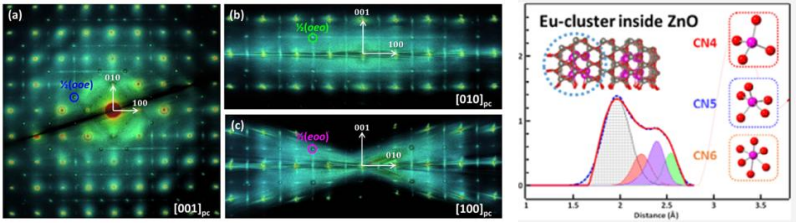

Figure 8. Left: Projection of 3D-ED of NBT-based ceramics showing diffuse scattering. Right: ePDF analysis of Eu-doped ZnO and the structural model.

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References:

[1] A. Neagu and C.-W. Tai, *Sci. Rep.*, 7, (2017), 12519
[2] D.T. Tran et al., *PJ. Appl. Cryst.*, 50, (2017), 304-312
[3] S. Feng et al., *Inorg. Chem.*, 64, (2025), 232-141

Local structure and dynamics in halide perovskites investigated with inelastic neutron scattering

M. Karlsson[1], R. Lavén[1], K. Shi[1], E. Fransson[2], P. Erhart[2], H. Cavaye[3], F. Juranyi[4], G.E. Granroth[5]

[1] Department of Chemistry and Chemical Engineering, Chalmers University of Technology, 412 96 Göteborg, Sweden
[2] Department of Physics, Chalmers University of Technology, 412 96 Göteborg, Sweden
[3] ISIS Pulsed Neutron and Muon Source, STFC Rutherford Appleton Laboratory, Chilton OX11 0QX, U.K
[4] Laboratory for Neutron Scattering and Imaging, PSI Center for Neutron and Muon Sciences, 5232 Villigen, Switzerland
[5] Neutron Scattering Division, Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, United States

Halide perovskites have emerged as technologically appealing materials for a vast array of optoelectronic applications. However, fundamental questions surrounding the local structure and vibrational dynamics remain to be elucidated for these materials. In this contribution, we will report on recent studies of the nature of local structure and vibrational dynamics in two halide perovskites, namely all-inorganic $CsPbI_3$ and organic-inorganic $MAPbBr_3$ (MA = methylammonium), using inelastic neutron scattering.

The study on $CsPbI_3$ [1] shows the material is characterized by a quasi-harmonic and almost temperature-independent lattice dynamics from 10 K all the way up to the orthorhombic-to-cubic phase transition at around 600 K. In the cubic perovskite phase (T > 600 K) of $CsPbI_3$, the dynamics are, conversely, highly anharmonic and overdamped, which are due to anharmonic rattling motions of the Cs^+ ions with the "perovskite cage" and spatially coherent, yet overdamped dynamics of the Pb-I perovskite sub-lattice. The study on $MAPbBr_3$ [2] exploited a unique light illumination kit to investigate the effect of the formation of photoexcited polarons on the INS spectrum and local structure. The results support previous findings by mid-IR spectroscopy, which suggests that light illumination leads to a local lattice distortion affecting the position and geometry of the MA cations with the perovskite lattice. These new insights can be expected to help in the rational design of new halide perovskites towards specific applications.

References:
[1] R. Lavén, E. Fransson, P. Erhart, F. Juranyi, G.E. Granroth, and M. Karlsson, *J. Phys. Chem. Lett.*, 16, (2025), 4812-4818
[2] K. Shi, H. Cavaye, R. Lavén, and M. Karlsson, *ACS Omega (In Press)*

Analysis of Ti and TiO_2 nanolayers irradiated with HCI Xe^{q+} using SR-GIXRF and SR-XRR methods

R. Stachura[1,2], P. Jagodziński[1,2], D. Banaś[1,3], A. Kubala-Kukuś[1,3], I. Stabrawa[1,3], K. Szary[1,3], G. Wesołowski[1], G. Aquilanti[4,*], I. Božičević Mihalić[5], I. Carlomagno[4], J.R. Herrera[4]

[1] Institute of Physics, Jan Kochanowski University, Uniwersytecka 7, 25-406 Kielce, Poland
[2] Central Office of Measures, Elektoralna 2, 00-139 Warszawa, Poland
[3] Holycross Cancer Center, Artwińskiego 3, 25-734 Kielce, Poland
[4] Elettra – Sincrotrone Trieste, s.s. 14, km 163.5 in Area Science Park, 34149 Basovizza, Trieste, Italy
[5] Rudjer Boskovic Institute, Bijenicka cesta 54, 10000 Zagreb, Croatia
[*] present address: The International Atomic Energy Agency, P.O. Box 100, Wagramer Strasse 5, A-1400 Vienna, Austria

Understanding of the structure and properties of nanolayers is essential for the development of advanced materials with tailored physical and chemical characteristics. One of the methods used to modify such materials is irradiation with low-energy highly charged ions (HCI), where both kinetic and potential energy deposition lead to the formation of surface nanostructures and changes in morphology [1]. In this work, titanium (Ti) and titanium dioxide (TiO_2) nanolayers deposited on Si substrates were irradiated with HCI (Xe^{q+}, q = 25–35) at Kielce EBIS facility (Jan Kochanowski University) [2]. The properties of irradiated nanolayers were characterized using synchrotron radiation-based X-ray reflectometry (XRR) and grazing incidence X-ray fluorescence (GIXRF) at the Elettra Synchrotron (Italy). XRR was applied to determine layer thickness, density, and interface roughness, while GIXRF provided depth-resolved information on elemental distribution [3]. The experimental data allowed evaluation of the influence of ion charge state on nanolayer morphology. The results show that irradiation leads to surface modifications, with changes in roughness and elemental distribution depending on the xenon ion charge state. Additionally, XRR data simulations using the XRRModeler software were performed in this work, enabling modeling and fitting of reflectivity curves in multilayer structures. This combined experimental and computational approach provides a comprehensive characterization of ion-irradiated nanolayers.

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References:
[1] J. Barth et al., *Nature*, 437(7059), (2005), 671-679
[2] Banaś D et al., *Nucl. Instrum. Meth. Phys. Res. B.*, 354, (2015), 125128
[3] R. Klockenkamper, A. Von Bohlen, John Wiley & Sons, (2014)

Curvilinear electronics: from geometry-induced magnetochirality to efficient THz converters

D. Makarov[1]

[1] Helmholtz-Zentrum Dresden-Rossendorf e.V., Bautzner Landstrasse 400, 01328 Dresden, Germany, d.makarov@hzdr.de

Physical properties of living but also synthetic systems in condensed and soft matter are determined by the interplay between the physical order parameter, geometry, and topology. Specifically to condensed matter, spin textures, static and dynamic responses become sensitive to bends and twists in physical space. In this respect, geometry effects emerged as a novel tool in various areas of physics to tailor electromagnetic properties and responses by adjusting curvature and 3D shape of thin films, 2D materials, and nanowires [1,2].

In this talk, we will address fundamentals of curvature-induced effects with the focus on magnetism including the possibility to tailor anisotropic and chiral magnetic responses and enabling novel nonlocal chiral symmetry breaking effects [3]. Recent highlights of the community include experimental proof of curvature-stabilized skyrmions [4], realization of twisted 3D racetracks [5], explorations on curvilinear altermagnets [6], tailoring solitons in curvilinear 2D magnets [7], curvilinear magnetoelectrics [8] to name just a few examples.

Beyond magnetism, curvature appeared as a powerful tool to tailor nonlinear electrical responses in nonlinear Hall materials with time-reversal symmetry [9,10]. The nonlinear Hall effect is at the basis of THz optoelectronic applications for the realization of efficient upconverters in 6G communication networks. On the specific example of 2D and 3D curvilinear Bi thin films, we will show that the strength of the nonlinear Hall effect can be controlled using an extrinsic classical shape effect: the geometric nonlinear Hall effect [11]. This endows the nonlinear Hall effect of Bismuth with the tunability encountered only in low-dimensional materials at low temperatures.

References:

[1] P. Gentile et al., *Nature Electronics* (Review), 5, (2022), 551-563
[2] D. Makarov et al., *Advanced Materials* (Review), 34, (2022), 2101758
[3] O.M. Volkov et al., *Nature Communications*, 14, (2023), 1491
[4] D.A. Gugato et al., *Nano Lett.*, 25, (2025), 8901-8908
[5] A.M.A. Farinha et al., *Nature*, 639, (2025), 67-72
[6] K. Yershov et al., *Phys. Rev. Lett.*, 134, (2025), 116701
[7] S. Jin et al., *Advanced Materials*, 37, (2025), 2501935
[8] C. Ortix et al., *Phys. Rev. Res.*, 5, (2023), L022063
[9] I. Sodemann et al., *Phys. Rev. Lett.*, 115, (2015), 216806
[10] Z.Z. Du et al., *Nature Reviews Physics* (Review), 3, (2021), 744-752
[11] P. Makushko et al., *Nature Electronics*, 7, (2024), 207-215

Enhancing the physical stability of amorphous pharmaceuticals through control of molecular mobility

M. Paluch[1]

[1] Institute of Physics, University of Silesia, 75 Pulku Piechoty 1, 41-500 Chorzow, Poland

The vast majority of solid drug formulations (e.g., tablets) contain active pharmaceutical ingredients (APIs) in a crystalline state. This preference arises from the high physical and chemical stability of crystalline forms, which ensures that their physicochemical properties remain unchanged over extended storage periods. However, a significant limitation of many crystalline APIs is their poor water solubility. This issue is substantial, as it is estimated that approximately 40% of marketed drugs and up to 75% of drug candidates in development exhibit low aqueous solubility.

One promising strategy to overcome this limitation is the conversion of crystalline APIs into disordered, amorphous forms, which typically exhibit enhanced solubility and bioavailability. Nevertheless, this approach introduces a critical drawback: amorphous systems are inherently physically unstable and prone to recrystallization during storage, leading to the loss of their advantageous properties [1].

This presentation will address strategies for improving the physical stability of amorphous APIs. Particular emphasis will be placed on the role of structural dynamics, which is widely recognized as a key factor governing stability in disordered systems. We will demonstrate that controlling molecular mobility can significantly enhance the physical stability of amorphous drugs. In addition, alternative approaches to inhibit recrystallization will be discussed.

References:

[1] M. Rams-Baron, R. Jachowicz, E. Boldyreva, D. Zhou, W. Jamroz, and M. Paluch, Amorphous drugs – benefits and challenges, Springer 2018

Decoupling between the structural and conductivity relaxation as a fingerprint of the ion transport mechanism

Z. Wojnarowska[1] and M. Paluch[1]

[1] Institute of Physics, University of Silesia in Katowice, 75 Pulku Piechoty 1a, Chorzow, Poland

The relationship between structural (α) relaxation and ionic conductivity (σ) relaxation governs charge transport in electrolytes. Here, we demonstrate that the degree of decoupling between these processes serves as a quantitative fingerprint for identifying ion transport mechanisms in ionic liquids (ILs), polymerized ionic liquids (PILs), and ionic composites. Through combined high-pressure dielectric spectroscopy and rheology, we reveal four distinct transport regimes: (1) In neat ILs, conductivity relaxation (τ_σ) strictly couples to structural relaxation (τ_α) with a Walden ratio of ~1, characteristic of vehicular transport; (2) In ILs revealing self-assembly the conductivity relaxation becomes much faster than the structural relaxation at T below the liquid-liquid transition point; (3) PILs exhibit partial decoupling due to frustrated ion-polymer interactions, but with conductivity reduced by 2–3 orders versus ILs; (4) IL-POSS nanocomposite with a high concentration of POSS nanoparticles reveal high viscosity while maintaining the conducting properties of the liquid state. Consequently, nanofluid is located above the ideal Walden line, i.e., in the superionic region. This provides a universal framework for classifying ion transport mechanisms based on their dynamic signatures, with immediate implications for solid-state batteries, where decoupled conduction is critical for combining high ionic conductivity with mechanical stability.

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References:

[1] Z. Wojnarowska et al., *J. Am. Chem. Soc.*, 137, (2015), 1157-1164
[2] Z. Wojnarowska et al., *Chem. Mater.*, 29, (2017), 8082-8092
[3] Z. Wojnarowska et al., *PRL*, 111, (2013), 225703
[4] Z. Wojnarowska et al., *J. Phys.: Condens. Matter*, 27, (2015), 073202
[5] S. Koymeth et al., *Nano Lett.*, 25, (2025), 9779-9786
[6] B. Yao et al., *ACS Appl. Mater. Interfaces*, 15, (2023), 39417-39425

Attuned Electronic Structure–Mismatched Phonon Structure (AES–MPS): A unified framework for engineering the electronic–phonon transport in thermoelectric materials

K.T. Wojciechowski[1]

[1] Thermoelectric Research Laboratory, Faculty of Materials Science and Ceramics, AGH University of Science and Technology, Al. Mickiewicza 30, 30-059 Kraków, Poland, wojciech@agh.edu.pl

The development of high-performance thermoelectric materials increasingly requires simultaneous control of charge and phonon transport. However, strategies that improve electronic transport often deteriorate thermal transport, while approaches designed to suppress phonon heat conduction frequently reduce carrier mobility. This fundamental trade-off motivates the search for new physics-based design principles.

The Attuned Electronic Structure–Mismatched Phonon Structure (AES–MPS) framework is presented as a unified methodology for engineering the Electronic–Phonon Transport Architecture (EPTA) of thermoelectric materials. Rather than optimizing the thermoelectric figure of merit through empirical modification of individual material parameters, AES–MPS proposes independent engineering of the electronic and phononic transport channels according to their respective physical mechanisms. The electronic subsystem is optimized through Fermi-level alignment, work-function matching, reduced interface resistance and high carrier mobility, whereas the phonon subsystem is designed by controlling elastic mismatch, interface thermal resistance (Kapitza resistance) and hierarchical phonon scattering across multiple length scales.

Originally developed within the framework of Effective Medium Theory for heterogeneous materials, the AES–MPS methodology has been experimentally validated in several classes of thermoelectric composites, including PbTe–$CoSb_3$, $Ge_{0.87}Mn_{0.05}Sb_{0.08}Te$–WC, $La_{0.95}Sr_{0.05}Co_{0.95}Mn_{0.05}O_3$–WC, $SrBi_4Ti_4O_{15}$–$La_{0.7}Sr_{0.3}MnO_3$, porous In–In_4Se_3, and polymer–tetrahedrite composites. In particular, the GeTe–WC composite reached ZT = 1.93 at 773 K, resulting from the synergistic combination of electronic compatibility and strong phonon scattering induced by acoustic impedance mismatch.

Beyond experimental validation, we will discuss the physical mechanisms governing heterointerface transport, residual thermal stresses, interface electronic states and multiscale phonon scattering. Finally, it will be argued that the concept of Electronic–Phonon Transport Architecture provides a general framework extending beyond composite materials towards rational design of next-generation thermoelectric materials based on independent engineering of electronic and phononic transport pathways.

References:

[1] A. Kosonowski et al., *J. Eur. Ceram. Soc*., 42, (2022), 2844-2852
[2] A. Kumar et al., *ACS Appl. Mater. Interfaces*, 14, (2022), 44527-44538
[3] A. Kosonowski et al., *Dalton Trans.*, 50, (2021), 1261-1273

Studies of magnetic properties of Eu compounds

D. Rybicki[1], K. Kowalczyk[1], K. Komędera[1], J. Przewoźnik[1], Ł. Gondek[1], Cz. Kapusta[1], W. Tabiś[1], M. Babij[2], L.M. Tran[2]

[1] AGH University of Krakow, Faculty of Physics and Applied Computer Science, al. A. Mickiewicza 30, 30-059 Kraków, Poland
[2] Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Okólna 2, 50-422 Wrocław, Poland

Europium-based compounds exhibit a wide range of intriguing properties due to the element's ability to exist in two valence states: Eu^{2+}, which carries a strong magnetic moment, and non-magnetic Eu^{3+}, as well as due to interactions between localized *f*-electrons and conduction electrons. During the presentation results on three compounds: $EuZn_2P_2$ [1], $EuZn_2As_2$ [2] and EuSnP [3] will be discussed. In order to understand Eu magnetism x-ray diffraction, heat capacity, AC and DC susceptibility, magnetization and Mössbauer spectroscopy (on ^{151}Eu) measurements were performed as a function of temperature and applied magnetic field. Proposed magnetic structures and their evolution with magnetic field will be discussed.

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References:
[1] D. Rybicki, K. Komędera, J. Przewoźnik, Ł. Gondek, Cz. Kapusta, K. Podgórska, W. Tabiś, J. Żukrowski, L. M. Tran, M. Babij, Z. Bukowski, L. Havela, V. Buturlim, J. Prchal, M. Divis, P. Kral, I. Turek, I. Halevy, J.Kastil, M. Misek, U. Dutta, and D. Legut, *Phys. Rev. B*, 110, (2024), 014421
[2] Z. Bukowski, D. Rybicki, M. Babij, J. Przewoźnik, Ł. Gondek, J. Żukrowski, and Cz. Kapusta, *Sci. Reports*, 12, (2022), 14718
[3] K. Podgórska, K. Komędera, J. Przewoźnik, Ł. Gondek, Cz. Kapusta, W. Tabiś, M. Babij, L.M. Tran, and D. Rybicki, *Sci. Reports*, 15, (2025), 30490

Understanding electric permittivity behavior in highly polar liquid crystal systems

M. Mrukiewicz[1], D. Węgłowska[2], M. Czerwiński[2], N. Podoliak[3], P. Perkowski[1], J. Szydłowska[4], D. Pociecha[4]

[1] Institute of Applied Physics, Military University of Technology, Kaliskiego 2, 00-908 Warsaw, Poland
[2] Institute of Chemistry, Military University of Technology, Kaliskiego 2, 00-908 Warsaw, Poland
[3] Institute of Physics, Academy of Science of the Czech Republic, Na Slovance 2, 182 00 Prague 8, Czech Republic
[4] Faculty of Chemistry, University of Warsaw, Żwirki i Wigury 101, 02-089 Warsaw, Poland

The discovery of the ferroelectric nematic phase (N_F) has revolutionized the study of soft matter polarity, offering a polar alternative to the classic nematic phase for use in advanced optical technologies. The scale of ferroelectricity in the N_F phase is very similar to that observed in solid ferroelectrics.

This presentation examines how molecular architecture specifically core substitutions and terminal moieties such as nitro, cyano, and fluorine groups determines the dielectric response and mesophase stability across several homologous series of rod-like compounds [1-3]. Interestingly, even a minimal structural change, such as the addition of a single methylene unit, can dramatically transform the material from a paraelectric to a ferroelectric state. The obtained experimental results from dielectric spectroscopy on the N_F, achiral ferroelectric smectic A (SmA_F) and C phase (SmC_F) phases show a complex polarization current (Figure 1a) and dielectric response (Figure 1b). The presence of the N_F phase is evidenced by the strong dielectric response of the collective mode. The relaxation mechanism is based on the rotation of molecules in-phase and anti-phase in adjacent ferroelectric domains. In smectics A_F and C_F, due to the layered structure, the relaxation mechanisms are different. The orthogonal SmA_F is characterized by a soft-type amplitude relaxation. Tilting of molecules in SmC_F causes the disappearance of the amplitude mode and detection of the phason mode, connected with the fluctuation of the azimuthal angle.

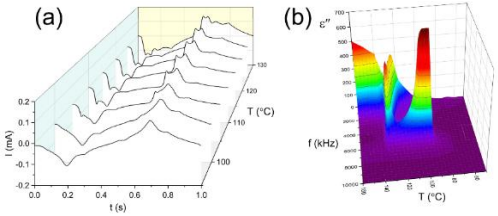

Figure 9 (a) Three-dimensional (3D) dependence on current peaks in the SmA_F and SmC_F phases. (b) 3D dependence of the imaginary part of electric permittivity (ε'') on temperature and frequency in achiral ferroelectrics.

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References:
[1] M. Mrukiewicz, M. Czerwiński, N. Podoliak, D. Repček, P. Perkowski, R.J. Mandle, and D. Węgłowska, *J. Mater. Chem. C*, 12, (2024), 7214-7224
[2] D. Węgłowska, M. Czerwiński, R. Dzienisiewicz, P. Perkowski, J. Szydłowska, D. Pociecha, and M. Mrukiewicz, *J. Mater. Chem. C*, 13, (2025), 9545-9553
[3] M. Czerwiński, M. Mrukiewicz, M. Filipow, D. Pociecha, N. Podoliak, D. Repček, M. Zając, and D. Węgłowska, *Chem. Mater.*, 37, (2025), 8077-8087

Submicron-precision machining of silicon surface with intense femtosecond extreme ultraviolet pulses

V. Lipp[1,2,3], G. Yamaguchi[4], S. Egawa[5], I. Inoue[6,4], K. Sakurai[7], D. Plakhuta[8], H. Noei[9], S. Toleikis[9], B. Ziaja[3,2]

[1] European XFEL, Holzkoppel 4, Schenefeld, 22869, Germany, vladimir.lipp@xfel.eu
[2] Institute of Nuclear Physics, Polish Academy of Sciences, Radzikowskiego 152, Kraków, 31-342, Poland
[3] Center for Free-Electron Laser Science CFEL, Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany
[4] RIKEN SPring-8 Center, 1-1-1 Kouto, Sayo, 679-5148, Hyogo, Japan
[5] Research Center for Advanced Science and Technology, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba, 277-8581, Japan
[6] Department of Advanced Materials Science, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba, 277-8581, Japan
[7] The Institute for Solid State Physics, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba, 277-8581, Japan
[8] Taras Shevchenko National University of Kyiv, Volodymyrska Street 64/13, Kyiv, 679-5148, Ukraine
[9] Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany

Femtosecond laser direct writing (LDW) using ultraviolet, visible or infrared lasers is a maskless subtractive manufacturing approach that is widely used for precision surface processing due to the strong spatial confinement of laser energy it provides and the minimal collateral damage it causes. Here, we present a conceptual scheme for high-precision machining of semiconductor materials using LDW with sub-micron-focused extreme ultraviolet (EUV) laser pulses. A proof-of-concept study was conducted at the SACLA free-electron laser facility, confirming the feasibility of the machining by creating reproducible craters with similar geometries in single EUV laser shots under fixed pulse parameters. The trends observed in the experiment were reproduced by theoretical simulations. These results clearly demonstrate the potential for controlled and reproducible semiconductor surface machining at the sub-micron length scale [1]. The proposed EUV LDW approach could pioneer transformative, cost-efficient manufacturing technology enabling direct, sub-micron- to nanometer-scale patterning of semiconductors and other technologically relevant materials.

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References:
[1] V. Lipp, I. Inoue, S. Egawa, K. Sakurai, et al., *submitted to Scientific Reports*

Visualizing spin waves with color center magnetometry

S. Mañas-Valero[1,2], Y.C. Doedes[2], A. Bondarenko[2], M. Borst[2], S. Kurdi[3], T. Poirier[4], J.H. Edgar[4], V. Jacques[5], Y.M. Blanter[2], T. van der Sar[2]

[1] Instituto de Ciencia Molecular (ICMol), Universitat de València, Valencia, Spain, samuel.manas@uv.es
[2] Department of Quantum Nanoscience, Kavli Institute of Nanoscience, Delft University of Technology
[3] Institute of Photonics and Quantum Sciences, SUPA, Heriot-Watt University, Edinburgh, United Kingdom
[4] Tim Taylor Department of Chemical Engineering, Kansas State University, Manhattan, Kansas, USA
[5] Laboratoire Charles Coulomb, Université de Montpellier and CNRS, Montpellier, France

Quantum sensing based on optically active spin defects (also known as color-center magnetometry) exploits electronic spins associated with atomic defects in solid-state materials, such as nitrogen vacancies in diamond and boron vacancies in hexagonal boron nitride, for quantitative nanoscale magnetometry with high sensitivity and spatial resolution. In this talk, I will introduce spin-wave sensing using color center magnetometry, specifically using color centers in diamond and hexagonal boron nitride to image spin waves at complementary frequencies.[1]

Spin waves (also known as magnons) in magnetic films have micrometer-scale wavelengths at gigahertz frequencies and are promising for wave-based information devices with new functionalities.[2] Realizing this promise requires accurate control of both the static magnetization and the spin-wave spectrum in microfabricated magnetic structures. In this context, quantum sensing with spin defects provides an excellent tool.

In particular, we harness the magnetic anisotropy in a permalloy magnetic half-plane to control the magnetic texture and excite spin-waves with highly field-tunable wavelengths. Via color-center magnetometry, we image both the static magnetic field generated by the magnetic texture and the dynamic fields generated by the spin-waves near the film edge. This enables us to determine the magnetic anisotropy, the magnetization curling length, and to correlate these with the spatially varying spin-wavelengths. Rotating the magnetic bias field, we trigger the non-reciprocal nucleation of a domain wall that strongly modulates the spin-wave transport near the film edge. Our results establish quantum sensing with optically active spin defects in solid-state materials as a versatile tool for advancing spin-wave technologies.

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References:
[1] S. Mañas-Valero et al., *Nature Comm.*, 17, (2026), 379
[2] S. Mañas-Valero et al., *Newton*, 1, (2025), 100018

Properties of DNA – surfactant complexes in thin films and bulk

M. Marzec[1]

[1] M. Smoluchowski Institute of Physics, Jagiellonian University, Prof. S. Łojasiewicza 11, 30-348 Kraków, Poland, monika.marzec@uj.edu.pl

Biopolymers such as deoxyribonucleic acid (DNA) have been the subject of intensive research in recent times due to their potential for applications outside the life sciences. DNA – surfactant complexes are particularly interesting because they are insoluble in water but soluble in alcohols and nonpolar liquids, so that their properties are not affected by humidity.

The aim of our study was to determine the influence of the distribution of DNA length and conformation as well as the surfactant structure on the properties of the complex in the form of bulk and a thin layer. Four types of DNA (three linear DNA, one plasmid DNA) and three cationic surfactants (cetyltrimethylammonium chloride – CTMA, benzyldimethylhexadecyl-ammonium chloride – BAC, hexadecylpyridinium chloride – HDP) were used to create complexes. We have shown that by the deposition DNA-CTMA complex on the solid substrate using the Langmuir–Blodgett method, linear structures are spontaneously formed most likely as a result of electrostatic and hydrophobic interactions between molecules [1]. It turns out that the structure of resulting monolayer depends on the compression conditions and the organization of molecules at the interface [2]. Moreover, the type of surfactant significantly affects the structure, degree of order and stability of complex [3] while the length, structure and type of DNA affect the organization of layer, its homogeneity and physicochemical properties [4]. Thus, the DNA type is important in the design of materials for applications as a thin layer in nanotechnology and optoelectronics. On the other hand, studies of DNA complexes in a powder form have shown that complexing DNA with surfactants leads to changes in spatial organization and their electric properties can be modified by selecting the surfactant and the length of DNA strand.

Summarizing, DNA-surfactant complexes represent a promising class of functional materials whose properties can be precisely controlled through the selection of components. Their self-assembly makes them attractive for applications in nanotechnology, materials engineering, and biomedicine.

References:
[1] J. Nizioł et al., *Polymer*, 178, (2019), 121643
[2] A. Radko et al., *Mat. Sci. & Eng. B*, 263, (2021), 114859
[3] A. Radko et al., *Polymer*, 235, (2021), 124277
[4] A. Radko et al., *Materials*, 18, (2025), 3022

Role of the transition metals in persistent luminescence phenomena

V. Boiko[1,2]

[1] Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Okólna 2, Wrocław, PL-50-422, Poland, v.boiko@intibs.pl
[2] Institute of Physics, National Academy of Sciences of Ukraine, 46 Prospekt Nauky, Kyiv, UA-03028, Ukraine

From the moment of the first publications to the present day, materials with long-lasting emission, known as persistent luminescence (PersL), have been of interest both from the point of view of fundamental science (trapping and de-trapping mechanisms, trap effects on the decay time etc.) and from the point of view of application in various fields of optics and sensors [1]. In these materials, transition metals are typically used as co-dopants to extend the decay time, and rarely as the sole dopant. One of the most studied was Cr [2] for which mechanisms of PersL have been studied in quite detail; for other transition metals (Fe, Ni, etc.), these processes remain poorly understood.

This study focused on the role of transition metals, specifically iron (Fe) and chromium (Cr), on the PersL of the $ZnGa_2O_4$ (ZGO) nanoparticles. Recent experimental findings from temperature-dependent spectroscopy have provided valuable insights into the excitation pathways associated with defects and trap-assisted recombination. The research particularly emphasises the differences in trapping and relaxation behaviours among various transition metals. Emission and excitation spectra recorded in the deep-ultraviolet (UV) range, extending up to 12 eV, enable a direct examination of high-energy electronic transitions associated with charge-transfer processes and defect states within the host lattice.

This combined spectroscopic analysis underscores the crucial role of transition metals in charge trapping, energy transfer to emission centres, and the resulting persistent luminescence. These findings deepen our understanding of the defect-mediated mechanisms that drive afterglow in ZGO and lay the foundation for rational defect engineering to enhance the performance of PersL materials.

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References:
[1] Y. Li et al., *Chem. Eng. J.*, 487, (2024), 150424
[2] N. Basavaraju et al., *PCCP*, 17 (2015) 1790-1799

Magnetocaloric effect in selected compounds with perovskite structure

M. Mihalik[1], M. Kovalik[1], I. Khan[1], M.F. Ashraf[1], M. Fitta[2]

[1] Institute of Experimental Physics, SAS, Watsonova 47, 0401 Košice, Slovakia
[2] Institute of Nuclear Physics, PAS, Radzikowskiego 152, 31-342 Krakow, Poland

The **magnetocaloric effect (MCE)** in perovskite-structured compounds ABO_3 is highly prized for solid-state magnetic refrigeration due to low processing costs, chemical stability, and highly tunable magnetic transition temperatures T_C. One part of our contribution is devoted to hole doped manganates $La_{1-x}Ag_xMnO_{3+\delta}$ exhibiting high magnetocaloric effect (MCE) in the vicinity of room temperature. Nowadays the interest shifts from classical ceramic materials to nano sized materials which can be used in biomedical application e.g. hyperthermia. Recently we studied MCE on $La_{0.80}Ag_{0.15}MnO_{3+\delta}$ nanoparticles with respect to the change of crystal structure from orthorhombic (*Pnma* space group) to rhombohedral (space group *R-3m*) [2] and our recent study of MCE on $La_{0.70}Ag_{0.25}MnO_{3+\delta}$ with rhombohedral crystal structure [3] revealed that the adiabatic temperature change ΔT_{max}, the change of magnetic entropy $-\Delta S_{max}$ and the relative cooling power RCP are maximal for sample treated in Ar and decrease with oxygen content.

Second part of our contribution focused on $RMnO_3$ single crystals where R = Nd and Gd presents the study of oxygen content and effect of Ti and Y substitution on the MCE in these systems. $NdMnO_{3+\delta}$, $GdMn_{1-x}Ti_xO_3$ ($0 \le x \le 0.1$) and $Gd_{1-x}Y_xMnO_3$ ($0 \le x \le 0.1$) compounds were synthesized by the floating zone method. Oxygen stoichiometry, controlled by growth atmosphere, critically dictates the structure, magnetism, and MCE of $NdMnO_{3+\delta}$. Negative magnetization at $T_{Comp} \approx 74.5$ K in the O_2-grown crystal and the distinct $-\Delta S$ features, including inverse MCE at ~ 6 K, underscore the sensitive Mn–Nd spin interplay. These results highlight oxygen-driven lattice rearrangements in the ac-plane as the key to the complex magnetic behavior of $NdMnO_{3+\delta}$ [4]. The system exhibits pronounced magnetic anisotropy resulting in a direction dependent of MCE. Ordering of Gd^{3+} ions induces an inverse MCE (positive value of $-\Delta S_M$) along the *b* and c-axes, while along *a*-axis only a normal MCE is observed. In the case of Ti doped crystals the magnetic entropy change displays a broad peak at $T_1 \approx 13$ K with $-\Delta S_M = 11.35$, 8.05, and 7.77 $Jkg^{-1}K^{-1}$ and corresponding relative cooling power (*RCP*) = 197.72, 164.70, and 166.78 Jkg^{-1} for $x = 0.0$, 0.05, and 0.1 under 5 T. A sharp $-\Delta S_M = 0.55$ $Jkg^{-1}K^{-1}$ (0.5 T) appears at $T_{lock} = 20$ K ($x = 0.0$), which shifts to higher temperatures with an applied magnetic field [5]. The large MCE at cryogenic temperatures in these compounds is promising for low-temperature magnetic refrigeration applications.

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References:

[1] M. Antoňak et al., *IEEE Trans. Magn.*, 50, (2014), 6800071
[2] M. Zentková et al., *Acta Phys. Pol. A*, 137, (2020), 900-903
[3] M. Zentková et al., *JMMM*, 549, (2022), 169002
[4] I. Khan et al., Proceedings 28th Conference of Slovak Physicists, (2025), 45-46
[5] M.F. Ashraf et al., Proceedings 28th Conference of Slovak Physicists, (2025), 43-44

Confinement driven non-collinear spin-textures in embedded nanomagnets

M. Krupiński[1], P. Sobieszczyk[1], M. Nord[2], R. Bali[3]

[1] Institute of Nuclear Physics Polish Academy of Sciences, Radzikowskiego 152, 31-342 Krakow, Poland
[2] Department of Physics, Norwegian University of Science and Technology, Trondheim 7491, Norway
[3] Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstraße 400, 01328 Dresden, Germany

Precise manipulation of spin-textures at the nanoscale is essential for the advancement in spintronic, neuromorphic, and quantum sensing technologies. It can be done with a direct magnetic writing using focused ion beams by locally transforming paramagnetic $Fe_{60}Al_{40}$ and $Fe_{60}V_{40}$ precursor alloys into ferromagnetic nanostructures [1]. In $Fe_{60}Al_{40}$ systems, lateral confinement during the writing triggers anisotropic lattice relaxation, which manifests as an additional magnetic easy axis [2]. This mechanism can be utilized in the ring-shaped structures, where the easy axis is distributed along a radius, stabilizing the magnetic non-collinear textures. On the contrary, $Fe_{60}V_{40}$ nanostructures reveal a distinct confinement-driven evolution of spin-textures as dimensions are reduced toward the nanoscale. While wider structures (>250 nm) exhibit Landau-like domains, the nanomagnets with sizes of 100 nm and smaller presents symmetric Néel-type domain walls with unusual configuration of magnetic moments at domain boundaries [3].

Experiments with directly written nanomagnets of various sizes and shapes allowed us to determine the stability ranges of available spin-textures accessible by focused ion beams. The magnetic microscopy results were supported by micromagnetic simulations, which successfully reproduced non-collinear magnetic structures and provided the phase diagram of stable and metastable spin-textures for rings and stripes. The study shows how magnetic anisotropy can be manipulated at the nanoscale leading to the formation of large variety of non-collinear magnetic configurations.

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References:
[1] R. Bali et al., *Nano Lett.*, 14, (2014), 2
[2] M. Nord et al., *Small*, 15, 52, (2019), 1904738
[3] Md. S. Anwar et al., *Adv. Funct. Mater.*, 35, (2025), e72721

Exploring photonic applications of luminescent electrospun polymeric fibers

Z. Korczak[1], K. Cyprych[1], M. Hancharova[1], A. Szukalska[1], D. Zając[1], L. Sznitko[1]

[1] Wroclaw University of Science and Technology, Faculty of Chemistry, Wybrzeze Wyspianskiego 27, 50-370 Wroclaw, Poland, lech.sznitko@pwr.edu.pl

Electrospinning is a simple and cost-effective processing technique that enables the production of polymeric fibers with diameters ranging from several tens of nanometers to several microns. This technique allows the formation of single fibers, yarns, or even freestanding fibrous mats [1]. Moreover, it can be easily scaled up to meet industrial requirements [2].

Typically, dense packing of small fibers can produce efficient light scattering. Moreover, if the fiber diameter is on the order of a light wavelength or larger, it also allows light to be wave-guided inside. Therefore, light transport through electrospun fibrous mats is of great interest, and electrospinning appears to be an effective approach for creating various types of disordered photonic materials. Finally, as a representative of wet-processing techniques, electrospinning enables straightforward functionalization by incorporating various dyes or colloidal nanoparticles, which can be added directly to the polymer solution prior to spinning. Thus, such fiber-based materials can be easily converted into functional luminescent systems that address the requirements of modern optoelectronics.

Here, we present the results of our research on functionalized polymeric mats containing various luminescent dyes. We investigate how electrospun materials can be used for downconversion in LED technology. We discuss how such integration can be used to control the resulting emission color. We also discuss how the alignment of electrospun fibers can affect the directionality of random laser emission. Finally, we show that the fiber density gradient in stacked hierarchical structures can be used to control the color of combined laser emission in accordance with the RGB color mixing principle.

References:

[1] J. Xue, T. Wu, Y. Dai, and Y. Xia, *Chem. Rev.*, 119, (2019), 5298-5415

[2] L. Persano, A. Camposeo, C. Tekmen, and D. Pisignano, *Macromol. Mater. Eng.*, 298, (2013), 504-520

Spintronic effects of chemisorbed aromatic cyclophanes

P. Kögerler[1,2], C. M. Schneider[2], M. Metzelaars[1,2,3]

[1] Institute of Inorganic Chemistry, RWTH Aachen University, 52056 Aachen, Germany. E-mail: paul.koegerler@ac.rwth-aachen.de
[2] Peter Grünberg Institute 6, Research Centre Jülich, 52425 Jülich, Germany
[3] current address: Department of Chemistry, University of Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland

Hybrids of organic molecules and ferromagnetic metal substrates, comprising controlled chemisorptive interactions, exhibit intriguing magnetic interfacial phenomena such as local magnetic hardening.[1] We aim to explore such features to expand the scope of spintronics device functionality from the molecular perspective, targeting molecular architectures that are specifically designed for magnetotransport measurements via scanning probe microscopy, and which can mimic e.g. spin valves. Diamagnetic pyrene-based cyclophanes define what is possibly the 'molecular sweet spot' for such hybrid systems, in that they provide virtually perfect frontier orbitals, functionalization options, thermodynamic stabilities and geometries.[2] In first studies on different 3d metals, these species indeed reveal surprising spin polarization effects.[3] This talk will summarize our current understanding and will provide an outlook what modifications are possible to such macrocycles, introducing chirality, magnetic anisotropy and redox activity.

References:
[1] M. Callsen, V. Caciuc, N. Kiselev, N. Atodiresei, and S. Blügel, *Phys. Rev. Lett.*, 111, (2013), 106805
[2] M. Metzelaars, S. Sanz, J. Rawson, R. Hartmann, C.M. Schneider, and P. Kögerler, *Chem. Commun.*, 57, (2021), 6660-6663
[3] M. Metzelaars, C.M. Schneider, J. Rawson, D.E. Bürgler, S. Sanz, F. Matthes, P. Kögerler, T. Hattori, S. Schleicher, and B. Borca, *Chem. Sci.*, 12, (2021), 8430-8437

Magnetic relaxation and ordering in single crystals of quasi-one dimensional $Co(NCS)_2(ligand)_2$ compounds

M. Foltyn[1], M.M. Rams[1], D. Pinkowicz[1], M. Böhme[2], W. Plass[2], C. Näther[3], M. Rams[1]

[1] Jagiellonian University, Kraków (Poland), m.rams@uj.edu.pl
[2] Friedrich-Schiller-Universität, Jena (Germany)
[3] Christian-Albrechts-Universitat, Kiel (Germany)

The family of $[Co(NCS)_2(ligand)_2]_n$ compounds is a playground to study magnetic relaxation of single chain magnets [1-3]. In these compounds, Co(II) ions are connected into chains by thiocyanate bridges that mediate strong ferromagnetic interaction. To every ion, there are also connected two ligands, which separate the chains from each other. However, between the chains, the magnetic interaction is still present, which together with the intrachain interaction causes the magnetic ordering in the range 3-8 K. The N_4O_2 environment of Co(II) produces a local anisotropy that in the ground Kramers state of Co(II) leads to effective Ising-like exchange interaction within $Co(NCS)_2$ chains. The interchain interaction is usually weak, and for that reason, single chain properties are observed, also in the ordered magnetic phase. We will present the comparison of two compounds from this family, with antiferromagnetic and ferromagnetic ground state, respectively. The monocrystal samples were prepared and studied using calorimetry, dc and ac magnetic measurements. These data are elucidated using micromagnetic Monte-Carlo simulations, ab initio calculations, and DMRG modelling. Relaxation times measured using monocrystal samples are much longer that those previously measured using powder samples. Additional relaxation process is clearly visible above the critical temperature, and it is temperature independent, which is unusual for single chain magnets.

References:
[1] M. Rams et al., *Chem. Eur. J.*, 26, (2020), 2837-2851
[2] M. Foltyn et al., *Phys. Chem. Chem. Phys.*, 24, (2022), 24439-24446
[3] J. Beyer et al., *Dalton Trans.*, (2026), doi:10.1039/D6DT00621C

Multifractal characteristics of liquid crystal textures

P. Oświęcimka[1], N. Osiecka-Drewniak[1], M. Piwowarczyk[1], R. Rak[2], E. Juszyńska-Gałązka[1]

[1] Institute of Nuclear Physics Polish Academy of Sciences, ul. Radzikowskiego 152, 31-342 Kraków, Poland
[2] Faculty of Exact and Technical Sciences, University of Rzeszow, Pigonia 1, 35-310 Rzeszów, Poland

Multifractality is one of the principal approaches for quantifying the structure of complex systems across a wide range of natural phenomena. In this study, we apply the multifractal formalism to analyze the complex structures of liquid-crystal textures in different phases. We show that the degree of multifractality serves as an effective measure of structural organization in liquid crystals, and that its temperature dependence exhibits behaviour analogous to a phase transition.

In particular, low-temperature smectic phases such as SmE and SmH display relatively simple textures with characteristics close to monofractality. Structural complexity increases progressively through the intermediate SmG and SmF phases, reaching its maximum in the SmI phase, which lies at the boundary between ordered and disordered regimes. This observation suggests that the highest degree of structural heterogeneity emerges near the onset of disorder.

Furthermore, we demonstrate a clear relationship between entropy changes associated with phase transitions and the degree of multifractal complexity. Transitions accompanied by small entropy changes produce only minor variations in complexity, whereas phases separated by large entropy increases exhibit a pronounced growth in multifractal complexity. These findings establish multifractal analysis as a powerful framework for quantifying structural complexity and tracking the evolution of order in liquid-crystal systems.

Symmetric and 2D-chiral hinged gratings: geometric limits, robust self-similarity and generalized conformability

P. Ulman[1], M. Święszek[1], D. Kuźma[2], P. Sobieszczyk[2], P. Zieliński[2]

[1] Faculty of Materials Science and Physics, Cracow University of Technology, Kraków, Poland
[2] Institute of Nuclear Physics, Polish Academy of Sciences, Kraków, Poland, piotr.zielinski@ifj.edu.pl

Proposed as examples of systems exhibiting negative mechanical response some star-like gratings have turned out exceptionally resistant to deformations of their central parts in that they regained their initial 4-fold point symmetry and self-similarity when far enough from their centres [1]. A reduction of symmetry from the 2D achiral point group 4m (D_4) to the 2D-chiral one 4(C_4) imposes unexpected limitations on the range of the parameters ensuring the existence and deformability of the stars [2]. The most interesting case is a complete rigidity of certain gratings in the limit of infinite number of self-similarity levels. A representation of the star geometry in the complex plane in analogy to conformal crystals [3] allows one to generalize the class of the objects to those showing variable self-similarity. Possible applications and perceptual consequences of the geometries under study will be discussed.

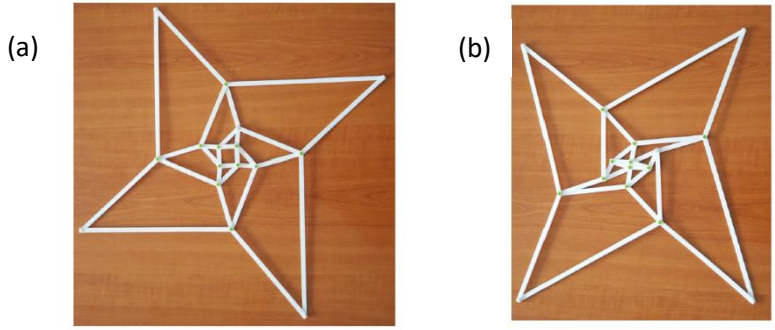

Figure 10. Model of four-arm 2D-chiral star in self-similar (a) and fully folded (b) state made with 3D printer by P. Ulman and M. Święszek..

References:
[1] P. Sobieszczyk, M. Mroczek, D. Kuźma, and P. Zieliński, *Phys. Status Solidi B*, 261, (2024), 2400399
[2] D. Kuźma, P. Ulman, M. Święszek, and P. Zieliński, *Phys. Status Solidi B*, 263, (2026), 70189
[3] F. Rothen and P. Pierański, *Phys. Rev. E*, 53, (1996), 2828

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    Controlling mesomorphism and glass transition in LC binary mixtures: the influence of composition and confinement

P1. Magnetic properties of Cu(II) monomer and trimer

R. Pełka[1], M. Fitta[1], J. Janczak[2], A. Wojciechowska[3]

[1] Institute of Nuclear Physics Polish Academy of Sciences, Radzikowskiego 152, 31-342 Kraków, Poland, Robert.Pelka@ifj.edu.pl
[2] Institute of Low Temperature and Structure Research Polish Academy of Sciences, Okólna 2, 50-422 Wrocław, Poland
[3] Faculty of Chemistry, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland

Magnetic properties of two novel molecular magnets based on Cu(II) ions are investigated. The first compound $[Cu(Hcda)(Im)(H_2O)]\cdot 0.5H_2O$ (**1**) (Hcda – monohydrated chelidamic acid, Im – imidazole) crystallizes in the monoclinic structure with space group C2/c and comprises pairs of Cu(II) monomers related by the inversion symmetry and coupled by the hydrogen bonds formed with the equidistant crystalline water molecule. The second compound $[Cu3(cda)_2(Im)_2(H_2O)_6]$ (**2**) crystallizes also in the monoclinic structure with space group $P2_1/c$ and consists of linear Cu(II) timers whose peripheral copper ions are related by the inversion symmetry. Magnetic measurements performed with the Quantum Design SQUID magnetometer indicate that **1** is a system of weakly interacting copper dimers coupled antiferromagnetically, while **2** comprises weakly interacting copper trimers with the antiferromagnetic intramolecular coupling. In both cases no long-range magnetic order was detected. The magnetic coupling between the dimer members of **1** (J = -1.26(1) cm^{-1}) seems to be mediated by the hydrogen bonds forming between the crystallization water molecule and the apical coordination water molecules. Interestingly, its magnitude is roughly twice higher than that observed between the peripheral Cu(II) ions and the central Cu(II) ion in the trimer of **2** (J = -0.655(5) cm^{-1}), although the coupling through the hydrogen bonds is usually expected to be weaker than that mediated by the coordination bonds. This may be due to the fact that the cda bridging moiety in the trimeric molecule is significantly spacious.

P2. Dielectric relaxation processes in liquid crystalline mixtures forming glass of tilted hexatic smectic phase

A. Deptuch[1], A. Drzewicz[1], M. Piwowarczyk[1], M. Pączek[2], M. Urbańska[3], E. Juszyńska-Gałązka[1,4]

[1] Institute of Nuclear Physics, Polish Academy of Sciences, Radzikowskiego 152, 31342 Kraków, Poland
[2] Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30387, Kraków, Poland
[3] Institute of Chemistry, Military University of Technology, Kaliskiego 2, 00908 Warsaw, Poland
[4] Research Center for Thermal and Entropic Science, Graduate School of Science, Osaka University, 560-0043 Osaka, Japan

Broadband dielectric spectroscopy (BDS) is applied to investigate relaxation processes in the smectic phases of six equimolar MHPOBC : 3FmHPhH6 (m = 2-7) mixtures, denoted as MIXmHH6, as well as of a ternary mixture consisting of MHPOBC : 3F2HPhH6 : 3F3HPhH6 in a molar ratio 0.5 : 0.25 : 0.25, denoted as MIX23HH6 [1]. All mixtures show enantiotropic SmA*, SmC*, and SmC_A* phases. Transition to a monotropic hexatic SmX_A* phase occurs at 302-312 K and the glass transition temperature of SmX_A* is 231-270 K, according to differential scanning calorimetry (DSC) results. For comparison, the corresponding temperatures for glassforming pure 3FmHPhH6 with m = 5, 7 are 283, 264 K and 247, 233 K [2,3]. The -C_mH_{2m}- chain length in a fluorinated 3FmHPhH6 component has a strong impact on relaxation processes in a supercooled state in mixtures. The α-relaxation time follows the Vogel-Fulcher-Tammann (VFT) dependence on temperature for MIXmHH6 with m = 6, 7, double VFT dependences for m = 3, 4, 5, and it merges with the secondary β-relaxation for m = 2, 2.5. T_g obtained from extrapolation of the α-relaxation time to 100 s is lower than T_g determined by DSC. At the same time, extrapolation of the relaxation time of the P_H phason from the SmX_A* phase to 100 s gives usually a better agreement with DSC results.

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[1] A. Deptuch et al., arXiv (2026), https://doi.org/10.48550/arXiv.2604.13653
[2] A. Deptuch et al., *Phys. Chem. Chem. Phys.*, 23, (2021), 19795-19810
[3] A. Deptuch et al., *Crystals*, 12, (2022), 1583

P3. From three dyes to two: simplified white random lasing with perylenes

A. Szukalska[1]

[1] Soft Matter Optics Group, Faculty of Chemistry, Wroclaw University of Science and Technology, Wybrzeże Stanisława Wyspiańskiego 27, 50-370 Wrocław

Lasers are typically monochromatic light sources emitting narrow spectral bands. In contrast, white lasing is a rare regime in which coherent emission spans the visible spectrum through balanced red, green, and blue components. Despite its nonmonochromatic character, it preserves key laser properties such as coherence, directionality, and high brightness, making it attractive for applications including high-resolution displays and Light Fidelity (Li-Fi) systems. [1,2]. A versatile approach to white light generation is random lasing (RL). Unlike conventional lasers requiring optical cavities, RL occurs in disordered media where feedback is provided by multiple scattering events. This cavity-free mechanism offers high flexibility in material design and emission tuning. Since 2015, numerous inorganic, organic, and hybrid white lasing systems have been demonstrated [3,4]. However, optimization of multicomponent gain media remains challenging, as precise control of energy transfer, spectral balance, and emitter distribution often requires complex architectures and time-consuming optimization procedures.

Here, perylene-based dyes are presented as promising gain materials for RL systems. Although widely explored in photocatalysis and organic solar cells, their lasing potential remains relatively underexplored. These derivatives exhibit high fluorescence quantum yields and excellent photostability. Moreover, their unique photophysical properties, including dual-band emission originating from coexisting dissolved and aggregated states, can significantly simplify white RL architectures. This multimodal behavior enables a transition from conventional three-dye systems to reduced two-component designs while maintaining efficient spectral tuning and white light generation [5].

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References:

[1] X. Zhan et al., *Adv. Mater.*, 33, (2021), 2104418
[2] H. Haas, *Rev. Phys.*, 3, (2018), 26-31
[3] A. Szukalska et al., *J. Mater. Chem. C*, 11, (2023), 8724-8757
[4] A. Szukalska et al., *Adv. Mater.*, 38, (2026), 1, e11648
[5] A. Szukalska et al., *Adv. Opt. Mater.*, 11, (2023), 16, 2300266

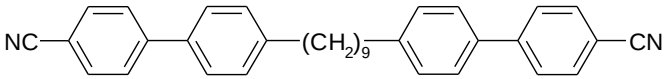
P4. Liquid crystal nematic twist-band phase in mixtures

M. Tykarska[1] and B. Klucznik[1]

[1] Military University of Technology, Institute of Chemistry, ul. Gen. Sylwestra Kaliskiego 2, 00-908 Warsaw, Poland, marzena.tykarska@wat.edu.pl

Nematic twist-band phase (N_{TB}) is a kind of liquid crystal phase formed by non-chiral compounds of a specific shape [1]. Two rigid elongated parts are connected by flexible alkyl chain. The typical example of such compounds CB9CB is presented in Fig. 1. Such molecules, called bimesogens, form macroscopic helical structure even though they are non-chiral compounds. The temperature range of such phase for single compounds is very narrow. One of the ways of lowering the melting points thus increasing the temperature range of existence of some phases is the preparation of mixtures.

We have performed the miscibility study to increase the temperature range of the existence of N_{TB} phase by mixing CBnCB, where n = 7, 9, 11, compounds with classical monomesogenic liquid crystal compounds. Two, three, and four ring compounds, having different terminal alkyl chain length and terminal polar group were tested. Some of the results were already published [2].



CB9CB

Figure 11. The chemical structures of a bimesogen CB9CB forming N_{TB} phase.

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References:
[1] M. Cestari et al., *Phys. Rev E*, 84, (2011), 031704
[2] M. Tykarska et al., *Materials*, 17, (2024), 4256

P5. Structural, thermal, and vibrational properties of glycine–chloranilic acid – a new complex

M. Brzostowicz[1], J. Hetmańczyk[2], Ł. Hetmańczyk[2]

[1] Jagiellonian University, Doctoral School of Exact and Natural Sciences, Prof. St. Łojasiewicza St 11, PL30348, Cracow, Poland, Jagiellonian University in Cracow, Faculty of Chemistry, Gronostajowa 2, 30-387 Cracow, Poland, monika.brzostowicz@uj.edu.pl
[2] Jagiellonian University in Cracow, Faculty of Chemistry, Gronostajowa 2, 30-387 Cracow, Poland

Chloranilic acid (CLA) is a proton donor that simultaneously exhibits electron affinity due to its quinoid structure, making it a suitable candidate for studies of hydrogen bonding and charge-transfer (CT) complexes, as well as their stability. Moreover, the presence of two equivalent –OH groups enable participation in supramolecular interactions [1]. It is well established that combining simple molecular systems, such as amino acids with organic compounds, can lead to the emergence of new physicochemical properties not observed in the individual components [2].

In this work, the glycine–chloranilic acid complex was investigated. At room temperature, the compound crystallizes in the triclinic system (space group P–1) and is isostructural with the N,N-dimethylglycine–chloranilic acid complex [1]. The polymorphic behavior and thermal stability of the system over a wide temperature range were examined using differential scanning calorimetry (DSC) and thermogravimetric (TG) analysis. DSC measurements revealed a reversible phase transition at 271 K upon heating and 249 K upon cooling. The observed thermal hysteresis of approximately 22 K, together with the sharp heat flow anomaly, indicates a first-order phase transition.

The entropy changes associated with the transition suggest significant configurational disorder in the high-temperature phase, characteristic of order–disorder (ODIC) crystals [3]. X-ray diffraction and NMR spectroscopy indicate the presence of protonated glycine species alongside deprotonated chloranilic acid dimers stabilized by strong O–H···O hydrogen bonds. The dynamic properties of the complex were investigated using temperature-dependent mid- and far-infrared spectroscopy (MIR and FIR), allowing the determination of activation energies for reorientational motions. Experimental IR spectra were compared with theoretical spectra calculated using density functional theory (DFT) under periodic boundary conditions (Quantum Espresso), showing good qualitative agreement. DFT calculations for isolated molecular models further supported the interpretation of vibrational features. Hirshfeld surface analysis was also performed to characterize intermolecular interactions and quantify key contacts within the crystal structure.

These findings provide comprehensive insight into the interplay between proton transfer, hydrogen bonding, and lattice dynamics, offering a deeper understanding of phase transitions in molecular charge-transfer systems.

References:
[1] J. Hetmańczyk, Ł. Hetmańczyk, W. Schilf, *Materials*, 14(12), (2021), 3292
[2] M. Zaman, M. Tomura, Y. Yamashita, *J. Org. Chem.*, 66(18), (2001), 5987-5995
[3] Dynamics of Solids and Liquids by Neutron Scattering, *Topics in Current Physics*, 3, (1977), S. W. Lovesey and T. Springer (eds.)

P6. ^{151}Eu Mössbauer spectroscopy and magnetic studies of EuAgAs single crystals

K. Kowalczyk[1], K. Komędera[1], J. Przewoźnik[1], Ł. Gondek[1], C. Kapusta[1], W. Tabiś[1], M. Babij[2], L.M. Tran[2], D. Rybicki[1]

[1] AGH University of Krakow, Faculty of Physics and Applied Computer Science, al. A. Mickiewicza 30, 30-059 Kraków, Poland
[2] Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Okólna 2, 50-422 Wrocław, Poland

EuAgAs is antiferromagnetic Dirac semimetal and crystallizes in hexagonal crystal structure ($P6_3/mmc$) [1-2]. In this compound europium magnetic moments order at 12 K [2]. Although some reports on this system exist, the magnetic characteristics of EuAgAs have not been fully explored yet. To gain deeper insight into its magnetic properties and ordering of europium's magnetic moments, the measurements of heat capacity, AC and DC susceptibility, magnetization and Mössbauer spectroscopy (on ^{151}Eu) were performed as a function of temperature and applied magnetic field. During the presentation, the detailed results of our study will be discussed.

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References:
[1] C. Tomuschat and H. Schuster, *Z. Naturforsch*, 36b, (1981), 1193-1194
[2] A. Laha et al., *Phys. Rev. B*, 103, (2021), L241112

P7. Examination of novel multicomponent systems of clotrimazole and organic acids for contemporary pharmaceutical challenges

M. Jamrógiewicz[1], G.P. Costa[2], F.J. Caires[2]

[1] Department of Physical Chemistry, Faculty of Pharmacy, Medical University of Gdańsk, Gdańsk, 80-416, Poland, majam@gumed.edu.pl
[2] School of Sciences, São Paulo State University, Bauru, 17033-360, SP, Brazil

The pursuit of well-being and quality of life motivates scientific research in the constant development of drugs. The key quality parameter, without which it is impossible to talk about the safety of using a drug, is physical stability, i.e. crystalline or amorphous structure, as well as chemical identity, characterized by the lack of degradation and changes in the composition of the sample [1]. However, the limited bioavailability and solubility of many active ingredients result in pharmaceutical forms that are difficult to administer, generating resistance in children, the elderly, and patients with specific needs. In this context, the formulation of multicomponent systems emerges as a technology capable of modifying properties without altering the original therapeutic effect [2]. This work presents the synthesis, physicochemical characterization, and solubility evaluation of new Clotrimazole's systems obtained with carboxylic acids in different proportions. This medicinal compound with the imidazole group is widely used for its antifungal spectrum and, recently, for its potential antitumor activity. However, its low solubility (0.49 μg mL^{-1}) places it in Class II of the Biopharmaceutical Classification System, requiring high dosages that can cause side effects [3]. There are obtained new systems (a eutectic mixtures, salts and amorphous) via vortex with minimal amounts of ethanol. The characterizations involved thermal (DSC), diffractometric (XRD), and spectroscopic analyses (FTIR/NIR), while solubility was validated by the shake-flask method. The results demonstrated optimized properties compared to the raw active compound, proving the potential of this technology to create materials that offer greater efficacy and convenience for the user.

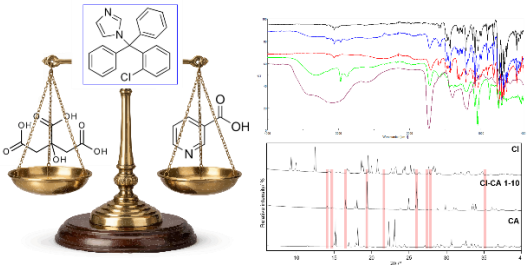

Figure 12. Proof-of-concept illustration of multicomponent system formation between clotrimazole and selected carboxylic acids. The scheme presents the concept of structural balance leading to new solid forms (eutectics, salts, and amorphous systems). Experimental evidence is provided by FTIR spectra, confirming intermolecular interactions, while complementary XRD patterns further support the formation of new solid phases with modified physicochemical properties.

Acknowledgments: This research was funded by Mayor of Gdańsk Fahrenheit Scholarship for International PhD Students.

References:
[1] O. González-González, I.O. Ramirez, B.I. Ramirez, P. O'Connell, M.P. Ballesteros, J.J. Torrado, and D.R. Serrano, *Pharmaceutics*, 14(11), (2022), 2324
[2] G.C. Bazzo, B.R. Pezzini, and H.K. Stulzer, *Int. J. Pharm*, 588, (2020), 119741
[3] S. Mittapalli, M.K.C. Mannava, U.B.R. Khandavilli, S. Allu, and A. Nangia, *Cryst. Growth Des.*, 15, (2015), 2493-2504

P8. Quantifying anharmonic effects on Raman spectra and thermal conductivity in β-$FeSi_2$ from first principles

S. Pastukh[1] and P. Piekarz[1]

[1] The Henryk Niewodniczański Institute of Nuclear Physics Polish Academy of Sciences ul. Radzikowskiego 152 31-342 Kraków, Poland, svitlana.pastukh@ifj.edu.pl

Iron silicides are promising materials for optoelectronic and thermoelectric applications [1], yet their thermal transport properties and the role of anharmonic effects remain not fully understood. In this work, we present a comprehensive ab initio study of lattice dynamics and phonon-mediated heat transport in the orthorhombic semiconductor β-$FeSi_2$.

Anharmonic effects are analyzed using both self-consistent phonon (SCPH) theory [2] and perturbation theory [3]. While SCPH yields only small renormalization of phonon frequencies, perturbative anharmonicity has a strong impact on phonon linewidths and selected optical modes. By combining Raman tensors with anharmonic phonon line shapes, we reproduce the temperature-dependent Raman spectra and resolve discrepancies with experimental linewidths.

Phonon lifetimes and group velocities are analyzed as functions of frequency, and the lattice thermal conductivity is evaluated over a broad range of temperatures and crystallite sizes. The results reveal weak anisotropy associated with the orthorhombic crystal structure and demonstrate that the third order anharmonic contributions play the dominant role in the thermal transport. The calculated thermal conductivity shows a good agreement with available experimental data, providing a consistent and validated description of heat transport in β-$FeSi_2$.

References:
[1] M.C. Bost, J.E. Mahan, *J. Appl. Phys*., 64, (1988), 2034-2037
[2] T. Tadano, S. Tsuneyuki, *Phys. Rev. B*, 92, (2015), 054301
[3] T. Tadano, S. Tsuneyuki, *J. Phys. Soc. Jap*., 87, (2018), 041015

P9. Controlling ion migration in argyrodites for stable thermoelectric devices

A. Rengarajan[1], M. Pindel[1], S. Sharma[1], O. Cherniushok[1], K. Wojciechowski[1]

[1] Thermoelectric Research Laboratory, Department of Inorganic Chemistry, Faculty of Materials Science and Ceramics, AGH University of Krakow, Mickiewicza Ave. 30, 30-059 Krakow, Poland, abinaya@agh.edu.pl

Controlling ion migration in Cu- or Ag-based argyrodites has emerged as a critical strategy for optimizing their thermoelectric performance, particularly due to the strong coupling between ionic transport and electronic conduction. Though tuning compositional disorder, lattice polarizability, and Cu-site occupancy can modulate the migration pathways and activation energy of mobile Cu ions. While material-level tuning is well explored, device-level implementation remains underdeveloped. In this work, we present a systematic design approach to engineer-controlled Cu-ion migration in argyrodites, aiming to enhance device stability and efficiency. The quantification of critical voltage (V_c) where ionic conductance exceeds baseline electronic leakage by >10% [1] has been performed in home-made four-probe set-up. The increased V_c is noticed for prepared argyrodites relative to binary analogues, explicitly arising from engineered defect landscapes that hinder Cu-ion migration. This enables suppression of detrimental ion drift under an applied electric field while preserving the intrinsically low lattice thermal conductivity characteristic of argyrodites [2]. A comprehensive understanding of ionic conductivity in argyrodites provides critical insights into the design and optimization of stable thermoelectric devices.

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References:

[1] K.A. Borup et al., *Energy Environ. Sci.*, 8, (2015), 423-435
[2] P. Taras et al., *Adv. Funct. Mater.*, 34, (2025), 2502163

P10. Pressure-induced spin-crossover in a 2D Hofmann clathrate studied by X-ray absorption spectroscopy

W. Sas[1], P. Konieczny[1], A. Pacanowska[1], A. Rogalev[2], F. Wilhelm[2], A. Maximenko[3], G. Gazdowicz[3], M. Fitta[1]

[1] Institute of Nuclear Physics Polish Academy of Sciences, Radzikowskiego 152, 31-342 Kraków, Poland, wojciech.sas@ifj.edu.pl

[2] ESRF – The European Synchrotron Radiation Facility, CS 40220, 38043 Grenoble, Cedex 9, France

[3] SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, ul. Czerwone Maki 98, 30-392 Kraków, Poland

Spin-crossover (SCO) compounds are prominent candidates in multifunctional materials because of their bistable nature and porous structures. Within this class, Hofmann clathrates – coordination polymers built from 2D $[M^{II}(CN)_4]^{2-}$ layers linked by organic ligands – stand out for their robustness. In contrast to many molecular systems, they typically exhibit isostructural transitions, where the framework remains preserved while bond lengths vary, enabling excellent cycling stability.

In this work, we investigate the pressure-induced SCO behavior in a 2D iron-nickel Hofmann clathrate: {[Fe(pyridazine)$_2$Ni(CN)$_4$]}, Fe(pdz)Ni, by X-ray absorption spectroscopy (XAS) using a diamond anvil cell (DAC). In particular, we study the evolution of the spin-state during the application of pressure within the range 0-1.04 GPa, and compare it to the temperature-driven spin transition at ambient pressure. The results show that Hofmann clathrates are promising candidates for sensitive pressure-temperature sensors.

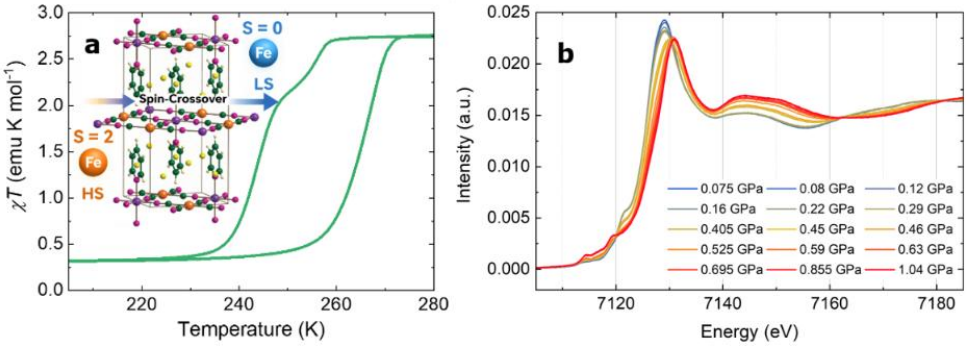

Figure 13. Magnetic susceptibility vs. temperature and crystal structure of Fe(pdz)Ni (a). Pressure-induced Fe K-edge XAS spectra of Fe(pdz)Ni (b).

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P11. The influence of the solvent on the preparation of different multicomponent solids of pioglitazone and tartaric acid

M.V. Porto[1], A.L. Almeida[1], B. De Maria[1], J.G. Santos[1], F.J. Caires[1]

[1] Faculty of Sciences, São Paulo State University (UNESP), Bauru, Brazil, mv.porto@unesp.br

Pioglitazone is a thiazolidinedione antidiabetic drug used to treat type 2 diabetes, characterized by its low solubility [1]. Studies of multicomponent solids, such as coamorphous systems, eutectics mixtures and salts, have shown promise in terms of optimizing of drug solubility. Coamorphous are non-crystalline, homogeneous systems formed by combining two or more low-molecular-weight components, with lattice disorder. Eutectic mixtures consist of two compounds that are bound by weak interactions, maintains the crystalline arrangement of the precursors while lowering the melting temperature. Salts, on the other hand, are formed by a reaction between an acid and a basic substance that involves proton transfer. This process requires ionizable groups [2,3]. This study examines the influence of solvent choice on the formation of different multicomponent solid forms between pioglitazone and tartaric acid, and the solids investigation. In this process, two mechanochemical approaches were employed: Neat grinding (NG) and Liquid-assisted grinding (LAG) using ethanol (EtOH) and methanol (MeOH). The resulting solids were characterized using FTIR, PXRD and DSC, revealing the formation of a coamorphous by NG, a eutectic mixture by LAG-EtOH and a salt by LAG-MeOH. The coamorphous form remained stable for up to 30 days before crystallizing in the eutectic obtained by LAGEtOH. Meanwhile, the optimal eutectic composition was studied using a binary phase diagram and Tamman's triangle. This revealed that the optimal eutectic ratio is 1:2. For the eutectic mixture (1:2) and the salt—stable and more promising forms—solubilities in an acid buffer were investigated. No changes in solubility were observed for the eutectic mixture, whereas the salt was 1.8 times more soluble than the pure drug.

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References:

[1] K. Shimada, et al., *Cryst. Growth Des.*, 25, (2025), 1514-1525
[2] A.C. Almeida et al., *J. Therm. Anal. Calorim.*, 150, (2025), 6885-6897
[3] J.G. Santos et al., *J. Mol. Struct.*, 1353, (2025), 144766

P12. Effect of Cr charge on trapping processes in Cr,Ca;YAG transparent ceramics

V. Boiko[1] and M. Chaika[1]

[1] Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Okólna 2, Wrocław, PL-50-422, Poland, v.boiko@intibs.pl

Yttrium Aluminium Garnet (YAG) transparent ceramics co-doped with Cr and Ca provide a model system for studying charge compensation and its effects on defect formation and carrier trapping. Incorporation of Ca^{2+} alters the charge balance, stabilising multiple chromium oxidation states (Cr^{3+}/Cr^{4+}) and influencing the population of intrinsic defects, such as oxygen vacancies and antisite defects, which act as trapping centres [1].

In this work, the effect of the chromium charge state, controlled by Ca co-doping, on trapping processes in Cr,Ca:YAG ceramics is investigated using Raman spectroscopy and thermoluminescence (TL). Raman analysis reveals local lattice distortions associated with changes in chromium valence and defect structure. TL measurements, performed after X-ray irradiation at varying doses and heating rates, provide information on trap depths, distributions, and kinetic parameters.

A correlation between chromium charge state, structural modification, and trap characteristics is established. The results show that Ca-induced charge compensation affects both the Cr^{3+}/Cr^{4+} ratio and the energetics of trapping centres. Based on combined Raman and TL data, a mechanism of charge trapping, de-trapping, and recombination involving chromium-related centres is proposed. These findings contribute to the understanding and control of trapping processes in YAG-based transparent ceramics.

Acknowledgements: This work was supported by the Polish National Science Centre, grant OPUS 23 Nr. UMO-2022/45/B/ST5/01487.

References:

[1] M.A. Chaika et al., *J. Chem. Phys.*, 151, (2019), 134708

P13. Low-temperature semiconductor-to-insulator transition in the $Ti/TiO_2/Fe$ system

J.C. Chojenka[1], A. Zarzycki[1], A. Vibhakar[2], A. Bombardi[2], M. Krupiński[1]

[1] Institute of Nuclear Physics Polish Academy of Sciences, PL-31342 Krakow, Poland, juliusz.chojenka@ifj.edu.pl
[2] Diamond Light Source Ltd, Harwell Science and Innovation Campus, Didcot, Oxfordshire, UK.

Titanium dioxide is a wide-band-gap semiconductor with promising properties for applications in energy storage, hydrogen generation, and photocatalysis. Moreover, TiO_2-based resistive switching devices offer significant potential for developing novel neural networks as artificial synapses. This is possible because TiO_2 exhibits a resistive switching effect, which occurs when it is sandwiched between two metallic electrodes. However, stoichiometric titanium dioxide can be readily reduced through chemical reactions at the interface with certain metals, such as W or Ni. This interaction at the metal–oxide interface facilitates the formation of a high concentration of oxygen vacancies, which in turn leads to the formation of TiO_2 suboxides.

To demonstrate the influence of titanium suboxides on the electrical properties of the $Ti/TiO_2/Fe$ system, we present results of our investigation of temperature-dependent resistance, correlated with the system's crystal structure. The resistance of the heterojunction exhibits three regimes: a single Schottky junction at high temperatures, a double Schottky junction at intermediate temperatures, and insulating behavior at low temperatures. The final regime corresponds to a transition to an insulating state at low temperatures, which is related to the reduction of TiO_2.

Our investigation revealed the presence of Ti_3O_5 and Ti_4O_7 phases. We suggest that the formation of these phases results from the reduction of TiO_2 at the interface with the iron layer, as well as enhanced internal stress at low temperatures. The formation of an insulating layer at the interface is responsible for the observed semiconductor-to-insulator transition.

P14. Balancing thermal robustness and physical stability: co-amorphous CBD–MEL systems under forced stress conditions

M. Mathew[1], J. Knapik-Kowalczuk[1], M. Paluch[1]

[1] Institute of Physics, Faculty of Science and Technology, SMCEBI, University of Silesia in Katowice, 75 Pułku Piechoty 1a, 41-500 Chorzów, Poland, mariya.mathew@us.edu.pl

Cannabidiol (CBD) is a pharmacologically active compound with broad therapeutic potential; however, its clinical application is significantly limited by poor aqueous solubility and low oral bioavailability. Amorphization is a promising strategy to enhance dissolution and apparent solubility, yet it is often constrained by poor physical stability and a strong tendency toward recrystallization. Although amorphous CBD shows relative stability under ambient conditions, it remains highly susceptible to pressure-induced recrystallization, underscoring the need for effective stabilization strategies.

A co-amorphous system combining CBD and melatonin (MEL) is explored as an approach to improve physical stability. MEL, a bioactive molecule with antioxidant and chronobiotic properties, is selected as a co-former based on its demonstrated potential in co-amorphous systems and its complementary pharmacological profile. Accordingly, co-amorphous CBD–MEL mixtures were prepared and characterized using thermogravimetric analysis (TGA), differential scanning calorimetry (DSC), and broadband dielectric spectroscopy (BDS). The eutectic composition was identified at CBD + 20% MEL based on experimental results supported by Schroeder–van Laar predictions. This composition exhibited the most favorable thermal properties and was therefore selected for high-pressure dielectric experiments.

The dielectric measurements performed under ambient and high-pressure conditions at 298 K demonstrate that the incorporation of 20% MEL significantly suppresses recrystallization and enhances the physical stability of amorphous CBD. These findings highlight MEL as an effective stabilizing co-former, supporting the development of robust co-amorphous formulations with improved pharmaceutical potential.

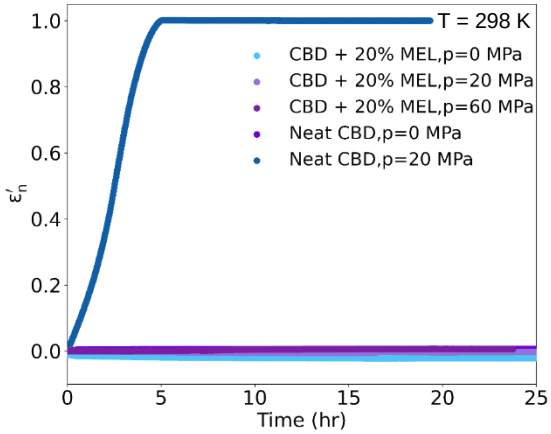

Figure 14. Crystallization Kinetics of Neat CBD and CBD + 20% MEL under ambient and elevated pressure at room temperature.

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References:

[1] M. Mathew, J. Knapik-Kowalczuk, M. Dulski, and M. Paluch, *Pharmaceutics*, 17, (2025), 358

P15. Probing charge transport in ionic liquid-POSS nano-hybrid electrolyte under extreme temperature and pressure conditions

S. Koymeth[1], M. Paluch[1], R. Cassalini[2], Z. Wojnarowska[1]

[1] Institute of Physics, the University of Silesia in Katowice, 75 Pułku Piechoty 1A, 41–500 Chorzów, Poland, Soorya.koymeth@us.edu.pl
[2] Chemistry Division, Naval Research Laboratory, 4555 Overlook Avenue Southwest, Washington, D.C. 20375, United States

Hybrid electrolytes combining ionic liquids (ILs) with nanoscale fillers offer a transformative route toward safe, high-performance energy storage; however, limited understanding of their charge transport under diverse environmental conditions hinders their application. We address this by examining the conducting, viscoelastic, and thermodynamic properties of a model quasi-solid electrolyte composed of an ammonium-based IL and charged polyhedral oligomeric silsesquioxane (POSS) nanoparticles over an extended temperature (173-393 K) and pressure (0.1-600 MPa) range.

By integrating PVT measurements with high-pressure dielectric spectroscopy, we quantify how the rigid POSS scaffold fundamentally reshapes the thermodynamic landscape of the host IL. The nanofiller creates a structurally reinforced, shear-thinning network that reduces compressibility and thermal expansion while maintaining efficient ion conduction via POSS-assisted percolation pathways. Notably, our high-pressure methodology allows us to decouple the roles of thermal energy and density on ion mobility. We report a profound shift in the conduction mechanism: while the neat IL transport is governed by both thermal activation and free volume ($\frac{E_V}{E_P} = 0.80$), dynamics in the IL-POSS composite are overwhelmingly dominated by thermal activation ($\frac{E_V}{E_P} = 0.95$).

Finally, we demonstrate for the first time in a nano-hybrid conductor the validity of the density-scaling concept. All conductivity data collapse onto a single master curve (γ=2.76), enabling accurate prediction of ion dynamics across 14 decades of frequency. This work provides a fundamental framework for tailoring nanohybrid materials for reliable operation in the extreme environments of next-generation batteries.

Acknowledgements: This research was funded in whole by the National Science Centre, Poland [Opus 21, 2021/41/B/ST5/00840].

References:
[1] S. Koymeth, M. Paluch, M. Dulski, Z. Wojnarowska, *Nano Lett.*, 25(24), (2025), 9779-9786

P16. Controlling rotating magnetocaloric response via magnetic anisotropy and topology in molecular systems

P. Konieczny[1], D. Czernia[2], R. Pełka[1]

[1] Institute of Nuclear Physics, Polish Academy of Sciences, Radzikowskiego 152, Krakow PL-31342, Poland, piotr.konieczny@ifj.edu.pl
[2] Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, Kraków, Poland, 30-387

Magnetocaloric performance in molecular materials is governed not only by the magnitude of the magnetic entropy change, but also by magnetic anisotropy, which enables a rotating magnetocaloric effect (RMCE) and can improve refrigeration efficiency.

In this contribution, we highlight a unified design strategy spanning anisotropic cyanide-bridged 2D ferrimagnets, Tb^{III}/Dy^{III} single-molecule magnets, and fluoride-bridged 3d-4f complexes. The earlier systems showed that RMCE can be self-enhanced by inverse magnetocaloric contributions along hard axes, reaching 51% enhancement in a Mn^{II}-Nb^{IV} ferrimagnet, while highly anisotropic Tb^{III} and Dy^{III} single crystals delivered RMCE maxima of 3.9 and 3.3 J kg^{-1} K^{-1} at 2.0 K under moderate fields. A quasi-2D Cu^{II}-W^{V} cyanido-bridged compound further demonstrated that conventional and rotating entropy changes can be tuned by crystallographic direction, with RMCE remaining significant near 38 K.

More recently, tetragonal 3d-4f fluoride-bridged complexes revealed switchable high-order anisotropy, showing that symmetry engineering can be used to design a new generation of molecular refrigerants. Together, these results establish anisotropy control, dimensionality, and topology as complementary tools for optimizing molecular magnetic cooling across cryogenic temperatures.

References:
[1] P. Konieczny, W. Sas, et al., *Dalton Trans.*, 51, (2022), 12762-12780
[2] P. Konieczny, D. Czernia, T. Kajiwara, *Sci. Rep.* 12, (2022), 16601
[3] L. Tacconi, A.S. Manvell, et al., *Angew. Chem. Int. Ed.*, 64, (2024), e202417582

P17. Testing the material time concept in nanoconfined glasses: equilibration kinetics of 5PPE in nanopores

Z. Pytlik[1] and K. Adrjanowicz[1]

[1] Institute of Physics, Faculty of Science and Technology, University of Silesia in Katowice, 75 Pulku Piechoty 1a, 41-500 Chorzów, Poland

Glassy materials undergo physical aging, changing their physical properties as they approach thermodynamic equilibrium. When confined in nanopores, glass-forming systems exhibit peculiar behavior, including out-of-equilibrium phenomena observed on a molecular timescale much faster than in the bulk. During equilibration, confinement-induced changes in the glass transition dynamics can be progressively eliminated. Recently, it has been demonstrated that a 'material time' concept can capture the out-of-equilibrium response of nanoscale confined glasses. Here, we test this framework for a model van der Waals liquid, 5-phenyl-4-ether (5PPE), confined within self-ordered nanoporous alumina templates of straight cylindrical nanochannels. We show that the equilibration kinetics can be successfully predicted for pores of different sizes and various thermal protocols. Our results provide new experimental evidence that the single-parameter aging concept remains valid not only for macroscopic glasses but also for nanoscale-confined glass-forming liquids.

References:

[1] Z. Pytlik, G. Mohandas, K. Skrzydelska, K.Chat, and K. Adrjanowicz, Testing the Material Time Concept in Nanoconfined Glasses: Equilibration Kinetics of 5PPE in Nanopores. (under review) (2026)

[2] K. Chat, E, Sikora, and K. Adrjanowicz, *J. Phys. Chem. Lett.* 16, (2025), 5076-5081

[3] K. Chat, K. Skrzydelska, E. Sikora, Z. Pytlik, and K. Adrjanowicz, *J. Mol. Liq.*, 433 (2025), 127859

P18. Interplay between relaxation dynamics and LC-like mesoscale organisation in amorphous POSA and ITRA: a multi-technique approach

G. Mohandas[1] and K. Adrjanowicz[1]

[1] Institute of Physics, Faculty of Science and Technology, University of Silesia in Katowice, 75 Pulku Piechoty 1a, 41-500 Chorzów, Poland, gopika.mohandas@us.edu.pl, karolina.adrjanowicz@us.edu.pl

The concept of liquid-crystalline (LC) ordering in amorphous pharmaceutical systems has attracted growing interest. In this regard, the azole antifungal drugs, including POSA and ITRA, due to the anisotropy of their molecules, can serve as excellent models for studying LC order in amorphous form. In the current study, we investigate the relationship between molecular dynamics and structure in these systems using dielectric spectroscopy, rheology, and atomic force microscopy (AFM). The relaxation behaviour is modelled as a superposition of Havriliak–Negami and Debye functions to account for the additional process. Rheological slope analysis further reveals deviations from classical terminal Maxwell behaviour in both POSA and ITRA. Stripe-like patterns observed in the AFM slope images, possibly linked to mesophase development in LCs, further support these conclusions. We also found that applying higher pressures changes the relaxation dynamics, likely due to penetrant-induced plasticisation, followed by additional densification during subsequent temperature scans. Interestingly, the stripe-like features disappeared after gas-pressure treatment, suggesting that the underlying ordering was disturbed. Overall, the present findings show the interplay between multicomponent relaxation dynamics and mesoscale orientational organisation in amorphous POSA and ITRA, providing further insight into hidden LC-like ordering phenomena in anisotropic pharmaceutical glass formers.

References:

[1] D. Heczko et al., *J. Phys. Chem. B*, 124, (2020), 11949-11961
[2] M. Rams-Baron et al., *Phys. Rev. E*, 104, (2021), 034702

P19. Role of interfacial interactions in the equilibration of DC704 confined in ALD-modified nanopores

K. Chat[1], M. Wojtyniak[2], Ł. Laskowski[1], E. Juszyńska-Gałązka[1], K. Adrjanowicz[3]

[1] Institute of Nuclear Physics, Polish Academy of Sciences, PL-31-342 Kraków, Poland
[2] Institute of Physics, Silesian University of Technology, Konarskiego 22B, 44-100 Gliwice, Poland
[3] Institute of Physics, University of Silesia, 75 Pułku Piechoty 1, 41-500 Chorzów, Poland

Non-equilibrium phenomena play a crucial role in determining the dynamics and stability of liquids under nanoscale confinement.[1,2,3] In this presentation, we investigate the glass transition dynamics and equilibration kinetics of tetramethyl tetraphenyl trisiloxane (DC704) confined within cylindrical anodic aluminum oxide (AAO) nanopores modified with Al_2O_3 and SiO_2 coatings prepared by atomic layer deposition (ALD). Using dielectric spectroscopy, we tracked changes in the α-relaxation time following temperature jumps of different magnitudes and directions and demonstrated that surface chemistry strongly influences both molecular mobility and equilibration behavior. In particular, SiO_2-coated nanopores exhibit faster dynamics but significantly longer equilibration times compared to Al_2O_3-coated pores, most likely due to stronger interfacial interactions and the formation of a thicker interfacial layer that limits molecular reorganization. Furthermore, the equilibration behavior of confined DC704 reveals the same characteristic features as physical aging in bulk glass-forming systems, including intrinsic isotherms, asymmetry of approach, and memory effects. Analysis within Narayanaswamy's material time framework shows that all normalized relaxation curves collapse onto a universal master curve when plotted as a function of reduced time, independent of thermal history, pore size, or surface chemistry. These findings confirm that the material time concept successfully describes nonequilibrium phenomena in chemically modified nanopore-confined systems and highlight the key role of surface interactions in controlling structural recovery under nanoconfinement.

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References:
[1] K. Adrjanowicz and M. Paluch, *Phys. Rev. Lett.*, 122, (2011), 176101
[2] K. Chat and K. Adrjanowicz, *J. Phys. Chem. C*, 124, (2020), 22321-22330
[3] K. Chat, E. Sikora, and K. Adrjanowicz, *J. Phys. Chem. Lett.*, 16, (2026), 5076-5081

P20. Influence of structure of two-ring core dopants on thermal stability of twist-bend nematic phase

B. Klucznik[1] and M. Tykarska[1]

[1] Military University of Technology, Kaliskiego 2, 00-908 Warsaw,
barbara.klucznik@wat.edu.pl

Nematic twist-bend (N_{TB}) phase is known since 2011, when it was experimentally confirmed [1]. This phase is built by non-chiral molecules, which form heliconical structure. Most of researchers are focused on searching new mesogens forming N_{TB} phase [2]. High melting points of compounds cause that N_{TB} phase is usually monotropic or enantiotropic in narrow range of temperatures. Making mixtures is the possibility to lower melting points. In few papers some information about results of miscibility studies in binary systems occur [3].

The aim of this work is the investigation of influence of structure of two-rigid core dopants (Fig.1) on thermal stability of twist-bend nematic phase in mixtures with CB9CB. Results indicate that changing the first benzene ring into cyclohexyl, dioxane and pyrimidine causes higher N-N_{TB} transition temperature. Irrespectively of the kind of ring, existence of N_{TB} phase is up to 0.7 mole fraction and is limited by inability to overcool samples to lower temperature without earlier crystallization.

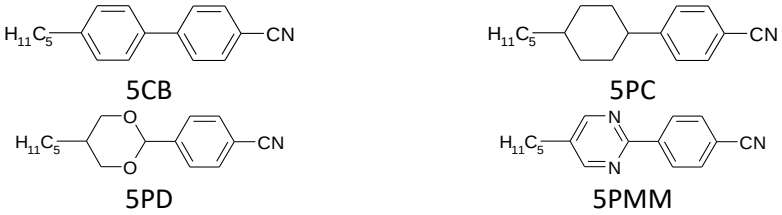

Figure 15. Tested compounds structures.

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[1] M. Cestari et al., *Phys. Rev E*, 84, (2011), 031704
[2] R. Mandle, Soft *Matter*, 12, (2012), 7883
[3] Z. Lu et al., *Liq. Cryst*., 41, (2014), 471-483

P21. Structural diversity of magnetic coordination polymers based on nickel complex and octacyanidometallates

M. Heczko[1] and M. Fitta[1]

[1] Institute of Nuclear Physics Polish Academy of Sciences, Kraków, Poland, michal.heczko@ifj.edu.pl, magdalena.fitta@ifj.edu.pl

Reactions performed between the cationic macrocyclic nickel(II) complex and anionic octacyanidometallates(IV) allow the formation of multiple coordination polymers that differ in the network building and geometry. The synthesis of new connections was carried out by self-assembly of building blocks in aqueous solutions, controlling the reaction temperature and introducing modifications in the form of the presence and amount of an additional electrolyte. It was possible to obtain a series of six 2D Ni-Nb coordination networks whose thermal stability and magnetic properties are dependent on the type of guest cations accommodated in the structure [1]. The research on Ni-Mo and Ni-W compounds shows the largest family of coordination polymers with cyanido bridges obtained from only one pair of building blocks. Moreover, the photomagnetic effect resulting from the excitation of octacyanidometallates forming coordination systems with nickel(II) ions was described for the first time [2]. The work also shows the topotactic reaction transforming straight Ni-Nb chains into the zigzag-shaped ones induced by temperature as well as the reverse process, which occurs upon increased humidity, which strongly changes the magnetic behaviour of those systems [3].

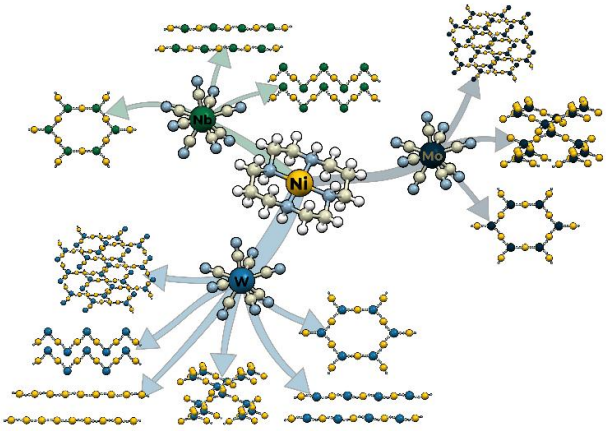

Figure 16. The scheme of reaction pathways leading to coordination networks characterized by different dimensionalities and topologies [1-3].

References:
[1] M. Heczko et al., *Dalton Trans.*, 50, (2021), 7537-7544
[2] M. Heczko et al., *Inorg. Chem.*, 61, (2022), 13817-13828
[3] M. Heczko, B. Nowicka, *Dalton Trans.*, 53, (2024), 5788-5795

P22. Pressure-induced molecular clustering in 3-phenylpropanal via π-stacking and distorted C–H···O hydrogen bonds

A. Krishna Sudhakaran Nair Valsala Kumari[1], B. Hachuła[2], P. Włodarczyk[3], M. Tarnacka[1], E. Kamińska[4], K. Kamiński[1]

[1] A. Chełkowski Institute of Physics, University of Silesia, 75 Pułku Piechoty 1, 41-500 Chorzów, Poland, anjana.krishna.s.v@us.edu.pl

[2] Institute of Chemistry, Faculty of Science and Technology, University of Silesia in Katowice, Szkolna 9, 40-006, Katowice, Poland, barbara.hachula@us.edu.pl

[3] Łukasiewicz Research Network – Institute of Non-Ferrous Metals, ul. Sowińskiego 5, 44-100 Gliwice, Poland, patryk.wlodarczyk@imn.lukasiewicz.gov.pl

[4] Department of Pharmacognosy and Phytochemistry, Faculty of Pharmaceutical Sciences in Sosnowiec, Medical University of Silesia in Katowice, Jagiellońska 4, 41-200 Sosnowiec, Poland, ekaminska@sum.edu.pl

High pressure is a powerful tool for directing molecular self-assembly because it reduces intermolecular distances without directly changing thermal energy. Here, we examine the pressure-controlled dynamics and association mechanism of the weakly associating aromatic aldehyde 3-phenylpropanal (3P1Pal), a good glass former whose supramolecular organization is visible in its dielectric response. Broadband dielectric spectroscopy reveals, besides the structural α-relaxation, a slower Debye-type process related to molecular clustering. Up to about 500 MPa, both relaxations exhibit nearly similar isochronal behavior; however, at higher compression the Debye mode shows a pronounced increase in amplitude and a growing time-scale separation from the α-process, indicating a pressure-induced change in the architecture of molecular associates. To clarify this unusual behavior, high-pressure FTIR and Raman spectroscopy were combined with molecular dynamics simulations. Vibrational spectra show pressure-induced shifts and broadening of aliphatic and aromatic C–H bands, while the carbonyl region displays a compensatory response caused by bond stiffening and stronger C–H···O interactions. Molecular dynamics simulations reveal that compression promotes larger and more compact aggregates than cooling. At low temperature, clustering is mainly governed by T-shaped π-stacking and nearly linear hydrogen bonds, whereas at high pressure mixed T-shaped/parallel π-stacking, formyl–formyl dipole correlations, and stronger but distorted C–H···O hydrogen bonds dominate. These findings demonstrate that pressure not only slows molecular mobility but also reorganizes the self-assembly pathway of 3P1Pal, offering molecular-level insight into pressure-tunable clustering in viscous molecular liquids [1].

References:

[1] A. Krishna et al., *J. Phys. Chem. Lett.*, 17, (2026), 728-736

P23. Crystalline polymorphism and melting of poly(dimethylsiloxane)

I. Tanizawa[1], K. Sugimoto[1], H. Suzuki[1]

[1] Department of Chemistry, Kindai University, Higashiosaka, Osaka 577-8502, Japan, Ib.tanizawa@gmail.com

Melting behavior of polymer differs from that of low-molecular-weight compounds, for example, in that crystalline and amorphous regions coexist, the melting temperature depends on crystal size, and recrystallization occurs during melting. Poly(dimethylsiloxane) (PDMS) is one of the well-known synthetic polymers, and its melting thermogram is known to consist of two endothermic peaks. However, crosslinked PDMS (CL-PDMS) exhibits single melting peak at a slightly lower temperature than that of uncrosslinked PDMS (UCL-PDMS).

In this study, to clarify the mechanism underlying the complex melting thermogram of PDMS, calorimetric (differential scanning calorimetry: DSC) and structural (temperature-dependent power X-ray diffraction: PXRD) measurements were conducted for UCL-PDMS and CL-PDMS. Figure 1(a) shows DSC heating curves for the three samples. As reported previously, UCL-PDMS exhibited two endothermic peaks (Peak I at 226 K, and Peak II at 238 K), while CL-PDMS showed one melting peak at 233 K. When UCL-PDMS was annealed at 229 K, Peak I disappeared, indicating that the crystalline state can be modified by annealing. Figure 1(b) shows the results of PXRD measurements, specifically the temperature dependence of the *d*-spacing corresponding to the (1 0 1) reflection. The *d*-spacing increased upon heating from 210 K to 226 K, then suddenly decreased above 226 K. The decrease ended at 230 K, after which the *d*-spacing began to increase again above 230 K. Upon annealing the sample at 232 K, this decrease disappeared, strongly indicating the presence of two polymorphic crystalline phases. For CL-PDMS, the *d*-spacing monotonically increased with temperature.

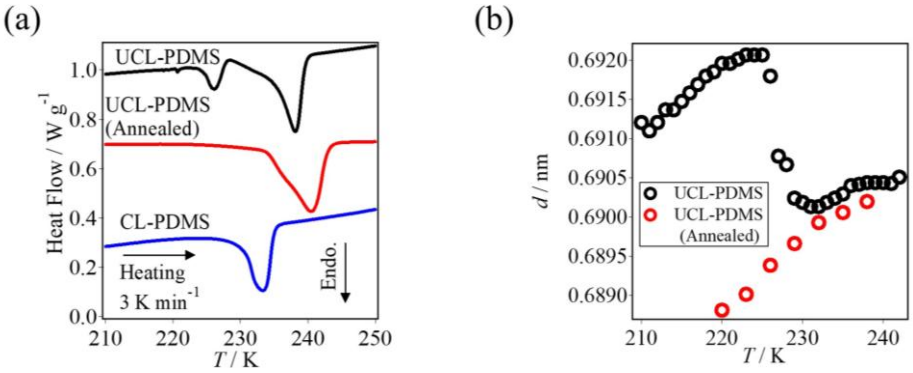

Figure 1. (a) DSC heating curves of UCL-PDMS, annealed UCL-PDMS and CL-PDMS. (b) Lattice spacings of (101) reflections for UCL-PDMS and annealed UCL-PDMS during heating.

P24. DFT calculation of temperature-dependent band gap renormalization in semiconductors

K. Tokár[1,2]

[1] Institute of Informatics, Slovak Academy of Sciences, Dúbravská cesta 9, 845 07 Bratislava 45, Slovakia, kamil.tokar@savba.sk
[2] Advanced Technologies Research Institute, Faculty of Materials Science and Technology, Slovak University of Technology, J. Bottu 25, 917 24 Trnava, Slovakia

Lead halide perovskites have emerged as transformative materials for next-generation optoelectronic and light-harvesting applications due to their exceptional tunable electronic properties [1]. In this study, we computationally investigated the temperature dependence of the electronic bandgap and sub-band states in case of orthorhombic $CsPb(I,Cl,Br)_3$ perovskite crystals across their phase stability range from 0 K to 400 K. Unlike conventional covalent semiconductors, these perovskites exhibit an anomalous blueshift of the electronic bandgap with increasing temperature. Our first-principles computational analysis attributes this behavior to the competition between thermal lattice expansion and robust electron-phonon coupling.

We demonstrate a predictive framework based on a standard Density Functional Theory (DFT) exchange-correlation approach to simulate the temperature-dependent electronic band structure. The framework models electron-phonon coupling using a series of displaced perovskite supercells sampled from a Bose-Einstein statistical distribution of a thermalized phonon system. The underlying lattice dynamics is determined using a direct approach utilizing DFT Hellmann-Feynman interatomic forces [2]. Notably, the simulated behavior of the electronic bandgap edge correlates with the dynamical contribution of the Urbach tail energy in optical spectra, yielding magnitudes that are highly compatible with experimental photoluminescence (PL) measurements [3].

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References:
[1] H.J. Snaith, *Nature Mater.*, 17, (2018), 372-376
[2] K. Parlinski, *Phys. Rev. B*, 98, (2018), 054305
[3] E. Ugur, M. Ledinsky, T.G. Allen, J. Holovsky, A. Vlk, and S. De Wolf, *J. Phys. Chem. Lett.*, 13, (2022), 7702-7711

P25. Competing magnetocrystalline and shape anisotropies as the origin of multistage remagnetization patterns in thin magnetic nanoparticles

H. Perepada[1], P. Zieliński[2], D. Kuźma[2]

[1] Faculty of Materials Science and Physics, Cracow University of Technology, Al Jana Pawła II 37, 31-864 Kraków, Poland
[2] Institute of Nuclear Physics Polish Academy of Sciences, Radzikowskiego 152, 31-342 Kraków, Poland, Dominika.Kuzma@ifj.edu.pl

Micromagnetic computations have been employed to model successive stages of magnetisation configurations in thin, planar, elliptical nanoparticles of hexagonal Cobalt. The easy axis of the material is aligned horizontally along the minor axis of the ellipse, i.e. perpendicularly to the vertical ellipse's major axis, which implies a competition between the magnetocrystalline and shape anisotropies. A variation of a magnetic field applied along the major axis entails either smooth or step-like changes of the overall magnetisation as a function of the size of the particle. The sizes at which the scenario of the remagnetization changes qualitatively define critical sizes [1]. Generally, the magnetisation stays in the plane of the particles if the size is small enough. The out-of-plane component of magnetisation, often in the form of spikes marking the vortex domain walls, appears for larger sizes. Figure 1(a) presents an example of pattern evolution with a varying external magnetic field in an elliptic nanoparticle. Figure 1(b) compares the analogous patterns in elliptic and rectangular shapes.

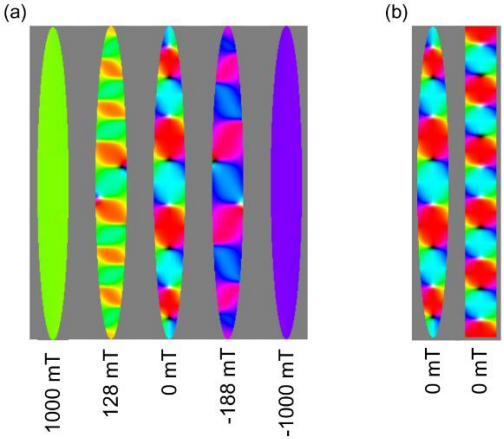

Figure 17. (A) Multiple stage remagnetization of a thin Cobalt nanoparticle with horizontal magnetocrystalline easy axis. (B) State with vortex domain walls in an elliptic and rectangular nanoparticle of equal outer size 80nm x 800nm x 20 nm.

References:

[1] D. Kuźma, L.M. Eng, and P. Zieliński, *J. Magn. Magn. Mater.*, 648, (2026), 174097
[2] D. Kuźma et al., *J. Magn. Magn. Mater.*, 545, (2022), 168685

P26. Modulated hard-soft ferromagnetic FeAl thin film fabricated with ion irradiation

A. Zarzycki[1], S. Anwar[2], R. Bali[2], K. Potzger[2], M. Krupiński[1], M. Marszałek[1]

[1] Institute of Nuclear Physics Polish Academy of Sciences, Radzikowskiego 152, 31-342 Kraków, Poland, arkadiusz.zarzycki@ifj.edu.pl
[2] Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstrasse 400, 01328 Dresden, Germany

The $Fe_{60}Al_{40}$ alloy exhibits a phase transition from a chemically ordered B2 crystallographic structure (characteristic of a hard ferromagnet with low magnetic saturation) to an A2 chemically disordered structure (characteristic of a soft ferromagnet with high magnetic saturation). This transition is readily achievable through methods such as thermal treatment or low-fluence ion irradiation. In our work, we irradiated a 40 nm thick $Fe_{60}Al_{40}$ alloy thin film with B2 structure, covered with a monolayer of self-assembled polystyrene (PS) nanospheres, using a broad Ne^+ ion beam at 25 keV and a fluence of 6×10^{14} ions/cm^2. Before irradiation, the PS nanosphere array was RF-plasma etched for varying durations to reduce the sphere diameter. In this way, we were able to fabricate magnetically modulated films with different area fractions of hard and soft ferromagnetic phases. Our main goal was the magnetic properties of these systems, which we investigated by combining DC and AC SQUID magnetometry measurements.

Our findings provide detailed insight into the magnetic composition of the irradiated (soft) and non-irradiated (hard) phases of the modulated systems. In particular, we were able to characterise the nature of the magnetic interactions between adjacent phases as a function of their relative volume. We observe exchange-spring magnet-like behaviour, in which the strength of the exchange coupling depends on the area ratio of irradiated to non-irradiated material. Furthermore, we identify strong magnetic inhomogeneity within the system, which gives rise to spin-glass behaviour at low temperatures, manifested by two distinct freezing temperatures associated with the irradiated and non-irradiated regions of the samples [1].

References:
[1] A. Zarzycki et al., *RCS Adv.*, 14, (2024), 36763-36770

P27. Magnetic excitation spectrum and hierarchy of magnetic interactions in $ErFeO_3$

D.R. Bhosale[1], P. Fabrykiewicz[1,2], D. Adroja[3,4], M. Meven[1,2], A. Schneidewind[1], M. Stekiel[1]

[1] Jülich Centre for Neutron Science at Heinz Maier-Leibnitz Zentrum, Forschungszentrum Jülich GmbH, Lichtenbergstraße 1, D-85747 Garching, Germany, m.stekiel@fz-juelich.de
[2] Institute of Crystallography, RWTH Aachen University, Jägerstraße 17–19, D-52066 Aachen, Germany
[3] ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, OX11 0QX, United Kingdom
[4] Highly Correlated Matter Research Group, Physics Department, University of Johannesburg, P.O. Box 524, Auckland Park 2006, South Africa

Rare-earth orthoferrites, $RFeO_3$ where R is a magnetic rare-earth ion, host two magnetic sublattices each governed by distinct energy scales, with the inter-sublattice coupling constituting a third, weaker scale. In particular, erbium orthoferrite with J=15/2 hosts Kramers degenerated 4f electron states, susceptible to perturbations [1] and giving rise to correlated magnetic effects, such as spin reorientation and spin switching [2].

We present a comprehensive investigation of the magnetic interactions in $ErFeO_3$, based on inelastic neutron scattering, in particular, neutron time-of-flight spectroscopy. Our measurements reveal a characteristic hierarchy of excitation energies in orthoferrites as well as the underlying hierarchy of magnetic interaction strengths. We characterize spin waves of the iron sublattice, crystal field (CEF) excitations of Er ions, splitting of the CEF levels, and spin-orbit coupling within iron sublattice, which together span the energy range from 100 to 0.1 meV [3].

Furthermore, we reveal the dispersive character of crystal field excitations of erbium, arising from Er-Er exchange coupling, and demonstrate the crucial role of dipolar interactions in the ground state splitting.

We present two theoretical frameworks: linear spin wave theory for spin waves and the Stevens formalism for CEF excitations, which are individually able to model the observed spectra, but cannot be straightforwardly unified. $ErFeO_3$ thus emerges as a vivid realization of multipolar magnetism, where spin and orbital degrees of freedom are deeply entangled. The observed hierarchy of interactions, and the limitations of existing theoretical frameworks, are likely universal features of the rare-earth orthoferrite family.

References:
[1] D.L. Wood et al., *Physical Review*, 185, (1969), 689-695
[2] I. Fita et al., *Phys. Rev. B*, 105, (2022), 094424
[3] D.R. Bhosale et al., *arXiv* 2604.27857, (2026)

P28. Spherical *vs* cubic palladium nanoparticles as potential nano-radiosensitizers in X-ray radiotherapy – *in vitro* studies

B. Klębowski[1], J. Courouble[2], O. Seksek[2], J. Depciuch[1], M. Parlinska-Wojtan[1]

[1] Institute of Nuclear Physics Polish Academy of Sciences, 31-342 Krakow, Poland
[2] IJCLab, CNRS UMR 9012, Universite Paris-Saclay, Université Paris-Cité, 91405 Orsay, France

Palladium nanoparticles (Pd NPs) are attracting increasing interest as a cost-effective alternative to gold-based nanostructures for biomedical applications, including radiosensitization [1,2]. In this work, we evaluated spherical palladium nanoparticles (Pd-Sph, **Figure 1a**) and cubic palladium nanoparticles (Pd-Cub, **Figure 1b**) as potential radiosensitizers for *in vitro* X-ray radiotherapy.

To improve cellular uptake and reduce toxicity, the Pd NPs were functionalized with thiolated glucose, exploiting the elevated glucose metabolism of cancer cells (Warburg effect) [3]. FTIR spectroscopy confirmed successful surface modification. Cytotoxicity and radiosensitizing potential were assessed using MTS assays, enabling the determination of critical concentrations that did not significantly reduce cell viability. Glucose-functionalized Pd-Sph and Pd-Cub showed improved biocompatibility, allowing the use of higher concentrations in subsequent irradiation experiments.

NPs–cells interactions were further investigated by label-free holotomographic microscopy. This technique enables real-time, three-dimensional imaging of living cells based on refractive index distribution, providing information on uptake dynamics, intracellular localization and morphology changes. The results demonstrated enhanced uptake of glucose-modified Pd NPs compared with non-modified systems. Pd-Cub showed slightly higher cellular internalization than Pd-Sph; however, no statistically significant differences in short-term radiosensitization were observed between the two shapes.

Overall, the study indicates that properly engineered Pd-Sph and Pd-Cub may serve as promising and economically attractive radiosensitizers for X-ray cancer therapy. Combining surface functionalization with advanced live-cell imaging provides valuable insight into NPs behavior and supports the future development of targeted nanomedicine strategies.

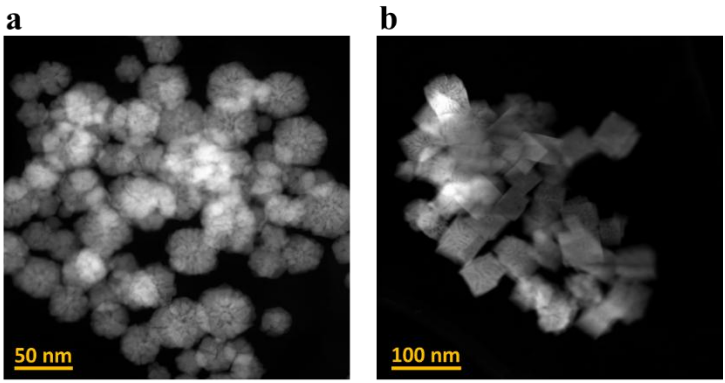

Figure 18. Representative STEM-HAADF images of Pd-Sph (a) and Pd-Cub (b).

Acknowledgements: The authors gratefully acknowledge the financial support provided under the PANCAKE project ,,**P**roton Therapy **A**ssisted by **N**ano Pd-DDS as **Ca**ncer Cell **K**ill**e**rs.

References:

[1] Y-W. Jiang, G. Gao, H-R. Jia, X. Zhang, X. Cheng, H-Y. Wang, P. Liu, and F-G. Wu, *Langmuir*, 36, (2020), 11637-11644

[2] B. Klebowski, A. Gałuszka-Bulaga, W. Komenda, J. Baran, and J. Depciuch, *ACS Appl. Nano Mater.*, 8, (2025), 22913-22926

[3] M. Jaworska, J. Szczudło, A. Pietrzyk, J. Shah, S.E. Trojan, B. Ostrowska, and K.A. Kocemba-Pilarczyk, *Pharmacol. Rep.*, 75, (2023), 876-890

P29. Thermal stability limits of Cu-based argyrodites: phase evolution and degradation in $Cu_8SiS_3Se_3$

S. Sharma[1], O. Cherniushok[1], T. Parashchuk[1], K. Pielichowska[2], K.T. Wojciechowski[1]

[1] Thermoelectric Research Laboratory, Department of Inorganic Chemistry, Faculty of Materials Science and Ceramics, AGH University of Krakow, 30-059 Krakow, Poland, ssharma@agh.edu.pl
[2] Department of Glass Technology and Amorphous Coatings, Faculty of Materials Science and Ceramics, AGH University of Krakow, Al. Mickiewicza 30, 30-059 Krakow, Poland

Cu-based argyrodites have attracted increasing attention as thermoelectric materials due to their intrinsically low thermal conductivity and promising electrical transport properties. However, their operational reliability is critically limited by insufficiently understood thermal stability, particularly under realistic environmental conditions. Here, we address this gap by introducing a quantitative framework for evaluating temperature-dependent stability and by establishing the operational limits of $Cu_8SiS_3Se_3$. We investigate phase stability, degradation pathways, and transport reversibility of $Cu_8SiS_3Se_3$ up to 873 K under inert (argon) and oxidative (air) conditions. High-temperature X-ray diffraction and thermogravimetric analysis are combined with cyclic transport measurements up to 773 K to directly assess structural and functional stability. To resolve degradation mechanisms, prolonged annealing at 873 K for 48 h is performed in vacuum and air, followed by cross-sectional SEM analysis to identify compositional gradients and volatile-element loss. Centre of this work, we introduce the Temperature Reversibility Index (TRI), a metric that quantifies the reversibility of transport properties during thermal cycling. We demonstrate that $Cu_8SiS_3Se_3$ maintains structural stability and reproducible transport properties only up to 473 K. Above this threshold, rapid degradation occurs. Under inert conditions, phase decomposition leads to $Cu_2(S,Se)$ and $Cu_2Si(S,Se)_3$, while exposure to air further accelerates degradation through oxidation, forming $CuSO_4$, Cu_2SO_5, and SiO_2. In both environments, selenium evaporation is the primary cause for degradation. TRI analysis provides a direct, quantitative measure of the collapse of transport reversibility and clearly shows the material's operational stability window. These results establish 473 K as the practical upper limit for reliable operation of $Cu_8SiS_3Se_3$ and identify the coupled effects of phase instability, oxidation, and volatile-element loss as the governing degradation mechanisms. More broadly, the TRI framework offers a generalizable tool for assessing stability limits in thermoelectric materials and enables more rational design of Cu-based argyrodites with improved thermal durability.

Acknowledgments: The research was supported by WEAVE-UNISONO 2022/04/Y/ST5/00139 project entitled “Entropy engineering and interface optimization in materials for highly effective thermoelectric energy conversion” funded by the National Science Centre, Poland. S.S.

References:
[1] T. Parashchuk, O. Cherniushok, B. Wiendłocha, J. Toboła, R. Cardoso-Gil, G.J. Snyder, Y. Grin, and K.T. Wojciechowski, *Adv. Funct. Mater.*, 35, (2025), 202502163

P30. Ferromagnetic resonance on patterned curvilinear permalloy surfaces

P. Sobieszczyk[1], J.C. Chojenka[1], M. Perzanowski[1], R. Bali[2], K. Potzger[2], M. Krupiński[1]

[1] Institute of Nuclear Physics Polish Academy of Sciences, Radzikowskiego 152, 31-342 Krakow, Poland
[2] Helmholtz-Zentrum Dresden-Rossendorf Institute of Ion Beam Physics and Materials Research, Bautzner Landstraße 400, 01328 Dresden, Germany

Ferromagnetic resonance (FMR) in patterned Permalloy ($Ni_{80}Fe_{20}$) structures has emerged as a powerful tool for probing spin dynamics in confined and curved magnetic systems. In Permalloy disks, the interplay between exchange and magnetostatic interactions gives rise to quantized spin-wave modes, including uniform, edge-localized, and vortex resonances, whose frequencies strongly depend on disk diameter, thickness, and magnetic configuration [1]. Extending FMR studies to curved and topographically modulated magnetic surfaces has revealed that curvature can significantly modify internal demagnetizing fields, induce anisotropic mode localization, and alter spin-wave propagation [2]. These effects are particularly relevant for emerging three-dimensional magnonic and spintronic architectures, where curvature-driven magnetic phenomena provide additional control over dynamic magnetic responses.

By using micromagnetic simulations we show how the hexagonal lattice arrangement of the permalloy disks changes FMR spectra and mode profiles in comparison with a single disk. Introducing the curvature of the surfaces changes magnetostatic energy of the system and gives rise to the additional branches of the magnonic spectra. The obtained calculations has been compared with experimental results.

Acknowledgements: Simulations were performed using the Polish high-performance computing infrastructure PLGrid (HPC Center: ACK Cyfronet AGH) for provided computer facilities and supported within a computational grant no PLG/2025/018615.

References:
[1] F. Guo. L.M. Belova and R.D. McMichael, *Phys. Rev. Lett*., 110, (2013), 017601
[2] J. Sklenar, P. Tucciarone, R.J. Lee, D. Tice, R.P.H. Chang, S.J. Lee, I.P. Nevirkovets, O. Heinonen, and J.B. Ketterson, *Phys. Rev. B*, 91, (2015), 134424

P31. Controlling mesomorphism and glass transition in LC binary mixtures: the influence of composition and confinement

M. Piwowarczyk[1], A. Deptuch[1], A. Drzewicz[1], O. Tomchuk[2], P. Jeleń[3], E. Juszyńska-Gałązka[1,4], Z. Galewski[5], M. Gałązka[1]

[1] The Henryk Niewodniczański Institute of Nuclear Physics Polish Academy of Sciences, Kraków (PL), presenting author e-mail: marcin.piwowarczyk@ifj.edu.pl
[2] ISIS Neutron and Muon Source, Rutheford Appleton Laboratory, Didcot (UK)
[3] Faculty of Materials Science and Ceramics, AGH University of Kraków, Kraków (PL)
[4] Research Center for Thermal and Entropic Science, Osaka University, Osaka (JPN)
[5] Faculty of Chemistry, University of Wrocław, Wrocław (PL)

Understanding phase behaviour in bulk and under spatial confinement is crucial for tailoring the physicochemical properties of multicomponent liquid-crystalline (LC) materials. Spatial confinement, such as electrospun fibres or nanoporous membranes, restricts molecular mobility and can strongly influence mesophase formation, vitrification, and crystallization processes.

A series of binary LC mixtures with varying molar compositions was prepared. The first component was a mesogenic azo compound from the (E)-4-((4-alkyloxyphenyl)diazenyl)phenyl alkanoates group (*n*OABOOC*m*, for n = 3, 5, 7, 8, 10, and m = 1 19) [1-3], while the second component was a chiral LC, cholesteryl pelargonate (PC). Selected mixtures containing PC exhibit glassy SmA* or crystalline phases. The influence of mixture composition on glass-forming ability, thermal stability, and phase formation is discussed.

Mesomorphic behaviour, thermal properties, dynamic processes, and structural organization were studied using Polarized Optical Microscopy, Differential Scanning Calorimetry, Broadband Dielectric Spectroscopy, and X-ray Diffraction. The observed phenomena include SmA* and crystalline glass formation, melt and cold crystallization, and double-step cold crystallization. Bulk studies were extended to spatially confined systems, including electrospun fibres and nanoporous membranes, using the same techniques complemented by Small-Angle Neutron Scattering and Fourier-transform Infrared spectroscopy. The results demonstrate that confinement significantly modifies mesophase behaviour and glass formation.

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References:

[1] M. Piwowarczyk, A. Deptuch, A. Drzewicz, et al, *Thermochim. Acta* 731 (2024) 179649
[2] M. Piwowarczyk, N. Osiecka-Drewniak, M. Gałązka, et al, *Phase Trans.* 92 (2019) 1066
[3] M. Piwowarczyk, A. Deptuch, A. Drzewicz, et al., *Liq. Cryst.*, 51, (2024), 2104-2116