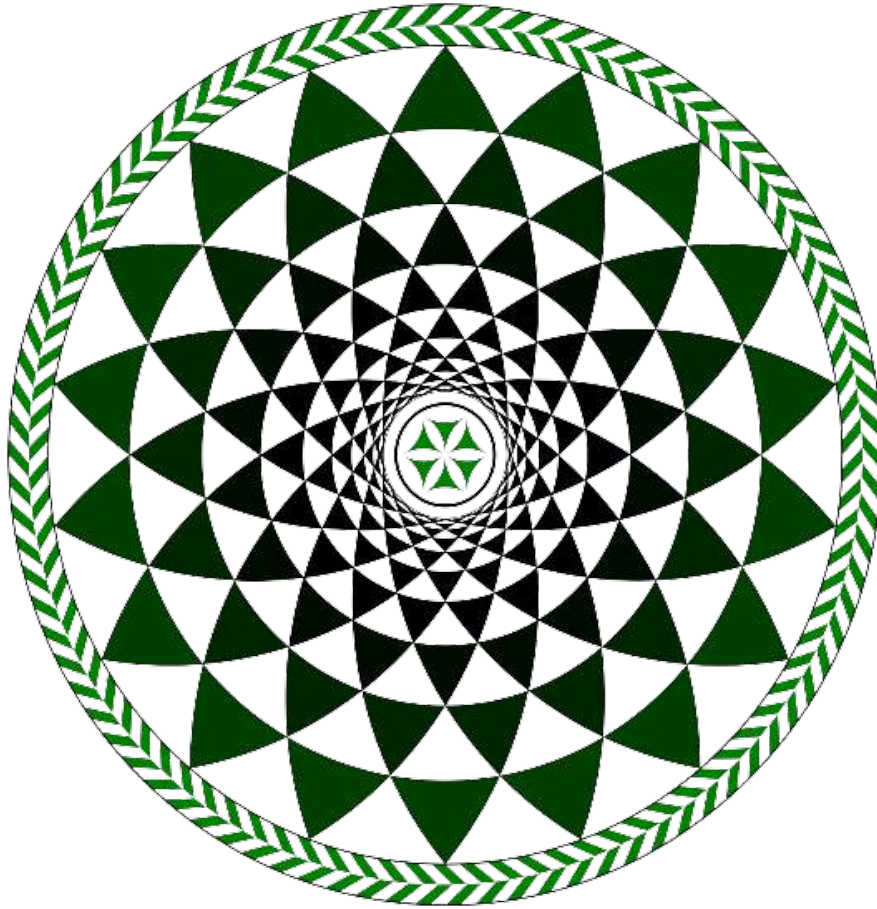


MULTIS 2024



Multiscale Phenomena in Condensed Matter

16 – 19 September 2024



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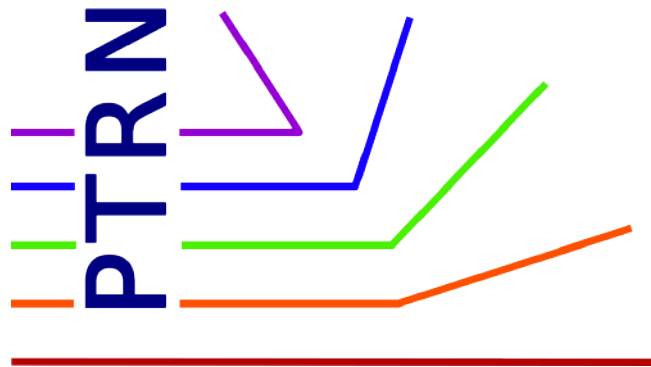
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PROGRAM OF THE CONFERENCE

MONDAY, 16 SEPTEMBER 2024

14:30	REGISTRATION	
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16:50	Opening lecture — Max Wolff (Uppsala, Sweden) Materials on the meso-scale	p.5
17:50	WELCOME PARTY	

TUESDAY, 17 SEPTEMBER 2024

Session: Soft matter and glass formers

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09:05	Mário Rosado (Coimbra, Portugal) Understanding intermolecular interactions in multicomponent solid phases with electronic structure calculations	p. 8
09:35	Hal Suzuki (Osaka, Japan) Calorimetric studies on phase transitions under shear flow for liquid crystal and colloidal system	p. 9
10:05	Aleksandra Pajzderska (Poznań, Poland) Computational insights on dynamics of 1-butyl-3- methylimidazolium tetrafluoroborate ionic liquid with different water concentration	p. 10
10:20	Taoufik Lamrani (Chorzów, Poland) Modification of the liquid-crystalline order in itraconazole using mechanical stress, temperature variation, and solvation	p. 11
10:35	COFFEE BREAK	

Session: Spectroscopic and diffraction methods

11:05	Serguei Molodtsov (Schenefeld, Germany) European XFEL: how does it work and fascinating applications	p. 13
11:40	Paweł Korecki (Kraków, Poland) Updates from SOLARIS national synchrotron radiation centre	p. 14
12:10	Cristian Svetina (Madrid, Spain) X-rays transient gratings at the european X-ray free electron laser	p. 15
12:40	Sebastião Antunes (Hamburg, German) Reconciliation of theoretical predictions and volume integrated ex- perimental data in ultrafast X-ray science through calculation of effective fluence	p. 16
12:55	Sara El Houbbadi (Kraków, Poland) Revealing the molecular structure of copper phosphonate groups anchored inside SBA-15 silica channels: theoretical and experi- mental study	p. 17
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Session: Multifunctional materials

14:30	Neven Žitomir Barišič (Wien, Austria) High- T_c cuprates – story of two electronic subsystems	p. 19
15:05	Yuki Utsumi Boucher (Zagreb, Croatia) Electronic and crystal structures of $\text{Eu}T\text{Ge}_3$ (T : transition metal) under extreme conditions	p. 20
15:35	Alessandro Surrente (Wrocław, Poland) Spin polarization dynamics in WSe_2 monolayer and in $\text{WSe}_2/\text{BAPbI}_4$ heterostructure	p. 21
16:05	Priyanka Reddy (Zagreb, Croatia) Murunskite: a bridge between cuprates and pnictides	p. 22
16:20	Serena Nasrallah (Fribourg, Switzerland) EuCd_2X_2 : semimetal illusion versus semiconductor reality	p. 23
16:35	COFFEE BREAK	
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17:35	Wojciech Tabiś (Kraków, Poland) Correlation between magnetism and the Verwey transition in magnetite	p. 25
	<u>Session: Flash talks</u>	
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18:09	Anna Janowska (Chorzów, Poland) Molecular dynamics simulations of the structure of amorphous pharmaceutical – probucol	p. 28
18:13	Sebastian Lalik (Kraków, Poland) An effect of small Au nanoparticle concentrations onto chosen properties in liquid crystal exhibits SmC_A^* phase	p. 29
18:17	Arkadiusz Zarzycki (Kraków, Poland) Unusual phase transformation kinetics in FePd thin films – inter-mediated phases and its magnetic properties	p. 30
18:21	Marcin Perzanowski (Kraków, Poland) Asymmetric magnetization reversal tailored by different oxidation procedures in Co/CoO exchange-biased thin films	p. 31
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18:37	Anna Drzewicz (Kraków, Poland) Self-assembly behavior of difluoroterphenyl derivatives differing with the linking bridge type	p. 35

18:41 **Marcin Piwowarczyk** (Kraków, Poland)
Investigation of phase behaviour and selective light reflection in mixtures with azo compounds p. 36

19:00 POSTER SESSION

WEDNESDAY, 18 SEPTEMBER 2024

Session: Molecular magnets and nanomagnets

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New opportunities for studying multiscale phenomena with neutrons p. 38

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09:35 **Marcin Sikora** (Kraków, Poland)
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10:05 **Illia Kozin** (Košice, Slovakia)
The field-induced Berezinskii–Kosterlitz–Thouless transition in a quasi 2D Heisenberg antiferromagnet $\text{Cu}[\text{C}_6\text{H}_2(\text{COO})_4][\text{C}_2\text{H}_5\text{NH}_3]_2$ on spatially anisotropic square lattice p. 41

10:20 **Bartosz Kłębowski** (Kraków, Poland)
The effect of cubic palladium nanoparticles (Pd NCs) surface modification on their cytotoxicity and radiosensitizing properties – in vitro studies p. 42

10:35 **COFFEE BREAK**

Session: Computational physics

11:05 **Pascal Simon** (Orsay, France)
Hund’s assisted multi-channel quantum phase transition in the $\text{Fe}(\text{Se},\text{Te})$ superconductor p. 44

11:40 **Dominik Legut** (Ostrava, Czech Republic)
Magnetostriction of polycrystalline terfenol-D – effect of grain morphology and orientation p. 45

12:10 **Natalia Osiecka-Drewniak** (Kraków, Poland)
Using neural networks to study liquid crystal textures p. 46

12:25 **Athanasios Koliogirgos** (Prague, Czech Republic)
An ab-initio theory of inelastic electron tunneling spectrum of vibrating magnetic molecules adsorbed on superconductors p. 47

12:40 **Ha Nguyen** (Kraków, Poland)
DFT study of optical properties and pressure dependence of electronic density of state in double perovskite $\text{Ba}_2\text{TiMnO}_6$ p. 48

12:55 **LUNCH**

14:30 **EXCURSION & CONFERENCE DINNER**

THURSDAY, 19 SEPTEMBER 2024

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- 08:30 **Javier Campo Ruiz** (Zaragoza, Spain)
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- 09:05 **Jan van Leusen** (Aachen, Germany)
About the magnetism of coordination compounds – from 3d to 5f metals p. 51
- 09:35 **Ján Titiš** (Trnava, Slovakia)
Advances in single-molecule magnets: investigating slow magnetic relaxation and its mechanisms p. 52
- 10:05 **Wiktor Wolański** (Kraków, Poland)
The new family of photomagnetic coordination frameworks based on $[\text{Mo}(\text{CN})_7]^{4-}$ building blocks p. 53
- 10:20 **Oliwia Polit** (Kraków, Poland)
Magnetic Ni@Au and Co@Au nanocomposite particles synthesised by laser ablation in liquid p. 54
- 10:35 **COFFEE BREAK**

Session: Miscellany

- 11:00 **Ubirajara van Kolck** (Trento, Italy)
The discrete charm of scale invariance p. 56
- 12:00 **Oleksandr Tomchuk** (Didcot, UK)
Structural organization of confined liquid crystals revealed by scattering techniques p. 57
- 12:30 **Adam Sieradzki** (Wrocław, Poland)
Hybrid Perovskites: exploring the thin line between order and disorder p. 58
- 13:00 **Grzegorz Dziembaj** (Kraków, Poland)
Few-body electron-hole photoluminescence spectra under the off-resonant THz-frequency laser beam irradiation p. 59
- 13:15 **Svitlana Pastukh** (Kraków, Poland)
First-principles analysis of anharmonic effects on thermal transport in graphene and h-BN p. 60
- 13:30 **LUNCH**

Session: Soft matter and glass formers

- 14:50 **Beata Nowicka** (Kraków, Poland)
Composites of a multistable and multiswitchable coordination chain p. 62
- 15:25 **Sebastian Pawlus** (Chorzów, Poland)
Supramolecular structures in monohydroxy alcohols: new group of halogen alcohols p. 63
- 15:55 **Yasuhiro Nakazawa** (Toyonaka/Osaka, Japan)
Hole-doped quantum spin liquid in Dimer-Mott organic compounds p. 64
- 16:25 **Daniele Sonaglioni** (Pisa, Italy)
PLX4720: new perspectives in an anticancer drug p. 65

16:40 **CLOSING REMARKS**

OPENING LECTURE, MON./16:50



Materials on the meso-scale

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In soft and hybrid materials the macroscopic properties are related to the structure and dynamics on the nano- and meso-scale. This provides large flexibility in the design of materials but is challenging for theory to describe, as a wide range of time and length scales are relevant. In materials physics at Uppsala University we focus on meta- and functional materials with an emphasis on non-equilibrium and finite size effects in amongst others magnetic materials, metal hydrides and soft matter. Samples are synthesised as well as studied in-house with e.g. x-rays, ions, optical methods and transport measurements. These characterisation tools are complemented by advanced x-ray and neutron scattering methods at large scale facilities. In this presentation I will highlight material systems, which can be well studied with neutron scattering methods.

The first example are polymer systems which are characterised by viscoelastic properties, which make them very interesting for applications in many areas of technology. The strong non-linearities in the response functions are related to the length and times scales on the molecular level and determined by the weak binding energies, which are close to ambient thermal energies. I will show results relating self-assembly as well as topological interactions in polymer systems to their viscoelastic properties. Apart from the changes in bulk properties, which are related to the molecular scale strong non-linearities may lead to macroscopic instabilities, such as shear banding or surface slip. In my presentation I will highlight surface scattering methods [1], which address a wide range of length scales and show that local ordering at interfaces is closely related to the topology and energy of interfaces as well as to shear.

As a second example I will present magnetic liquids, which provide large flexibility for tuning the interaction between the constituents. This allows to control self-assembly and the formation of defined structures in a bottom-up approach. Depending on the shape, size and moment of the magnetic particles the self-assembly process may result in ordered crystalline or defect rich open network structures [2]. In this presentation I will summarise results on the phase formation in a two-dimensional binary magnetic liquid and discuss possibilities for layer-by-layer deposition on solid substrates [3].

[1] M. Wolff, EPJ Web of Conferences, 188, (2018), 04002.

[2] H. Carstensen *et al.*, Soft Matter, (2022), 18, 6222.

[3] A. Saini *et al.*, Langmuir. 37, (2021), 4064.

SOFT MATTER AND GLASS-FORMERS

Chair: Pascal Simon

08:30	Silvina Cervený (San Sebastián, Spain) New findings of the glass transition of confined water	p. 7
09:05	Mário Rosado (Coimbra, Portugal) Understanding intermolecular interactions in multicomponent solid phases with electronic structure calculations	p. 8
09:35	Hal Suzuki (Osaka, Japan) Calorimetric studies on phase transitions under shear flow for liquid crystal and colloidal system	p. 9
10:05	Aleksandra Pajderska (Poznań, Poland) Computational insights on dynamics of 1-butyl-3-methylimidazolium tetrafluoroborate ionic liquid with different water concentration	p. 10
10:20	Taoufik Lamrani (Chorzów, Poland) Modification of the liquid-crystalline order in itraconazole using mechanical stress, temperature variation, and solvation	p. 11

KEYNOTE, TUE./08:30



New findings of the glass transition of confined water

S. Cervený^{1,2}

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Understanding the properties of strongly confined water (2-3 nm) is essential for various applications, such as desalination devices or voltage generation. In addition, confined water also plays a critical role in biological processes, such as flow through ion channels. Moreover, water under confinement can be supercooled without crystallization. Therefore, experiments at low temperatures on confined water in slits of 2-3 nm can shed light on properties such as the glass transition temperature (T_g), which has been the subject of intense scientific debate over the last twenty years.

Early adiabatic calorimetric experiments of water confined in nanopores of silica glass found a glass transition temperature (T_g) of 170 K, results questioned by Johari *et al.* [2]. These observations have not been generalized to other types of confinements, resulting in minimal experimental evidence of the glass transition of confined water.

This talk will first review the glass transition and the dynamics of bulk and confined water at supercooled temperatures. Then, using standard (DSC) and fast scanning calorimetry (FSC) measurements, we will reveal that water confined in MCM-41 and molecular sieves (MS) of different pore sizes shows a complex heat capacity behavior [3]. Through annealing experiments in the glassy state, we provide clear evidence that T_g of confined water is located at temperatures between 170 and 200 K, depending on the confinement. In addition, we show the presence of an extra low-temperature endotherm, identified with a sub- T_g thermal event, also addressed as a shadow glass transition in the temperature range 120-130 K. Finally, a high-temperature step in the heat capacity is also observed at temperatures above T_g , insensitive to annealing and, therefore, attributed to a proper thermodynamic transition. Finally, we will discuss the implications of these findings on the dynamics of confined and bulk water.

[1]

[1] A. Nagoe *et al.*, J. of Phys. Chem. B, 114, (2010) 13940-13943

[2] E. Tombari & GP Johari. J. Chem. Phys. 139,(2013), 064507

[3] J. H. Melillo *et al.*, submitted (2024)

INVITED TALK, TUE./09:05



Understanding intermolecular interactions in multicomponent solid phases with electronic structure calculations

M. T. S. Rosado , J. F. C. Silva , and M. E. S. Eusébio

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Multicomponent solid phases have broad application in the fields of pharmaceuticals and materials, enhancing or tune the properties of crystalline (cocrystals) or amorphous solid phases (co-amorphous). Most frequently, the aggregates of different compounds are stabilized by hydrogen bonding, but sometimes by halogen bonding, π -stacking, and other kinds of intermolecular interactions. Their analysis and characterization are usually performed by spectroscopic, calorimetric and X-ray diffraction techniques. Nevertheless, computational chemistry methods based on electronic structure calculations can provide a more fundamental insight.

Most, if not all, interactions among different molecules in solid phases have a fundamentally electrostatic nature. Therefore, the calculation of the electrostatic potential of isolated molecules of each component can provide insights into the possible interactions, often with predictive capabilities. A modification of previously proposed methods based on H-bond donor/acceptor strengths, enhanced with the use of available experimental data, is proposed and demonstrated for select systems.

The interactions in the aggregates of different molecules that are the fundamental structural units in the solid phases can be studied by electronic structure methods like Non-Covalent Interactions (NCI), the Independent Gradient Model (IGM- δg) and Natural Bond Orbitals (NBO). Even lacking complete structural resolution by diffraction methods, available experimental results can guide the calculations for the analysis of selected molecular aggregates.

Acknowledgements: CQC-IMS is funded by Fundação para a Ciência e Tecnologia (FCT) projects with DOI identifiers 10.54499/UIDB/04564/2020, 10.54499/UIDP/04564/2020.

INVITED TALK, TUE./09:35

Calorimetric studies on phase transitions under shear flow for liquid crystal and colloidal system

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Liquid crystals and colloidal systems are known to exhibit shear induced transitions (SITs), indicating that the thermodynamic stabilities are affected by the shearing. In this study, for the purpose of evaluating those effects experimentally, we have developed a differential scanning calorimeter equipped with a shearing system (Shear-DSC) [Fig. 1(a)], and investigated a thermotropic liquid crystal 8CB, and a cationic surfactant CTAB aqueous solution [1, 2].

For 8CB, the heat flow curves intrinsic to the transitions were successfully obtained by subtracting the contribution of shearing heat [Fig. 1(b) and (c)]. It was revealed that the onset temperature of SmA-N transition slightly shifts to lower temperatures with increasing shear rate. For CTAB aqueous solution, temperature of the transition from CTAB crystal to the rod-like micellar phase was found to change with shearing rate, which was attributed to the orientational ordering of micelles as well as the fracturing of crystallites. For both systems, the changes of transition entropies were found to be very small.

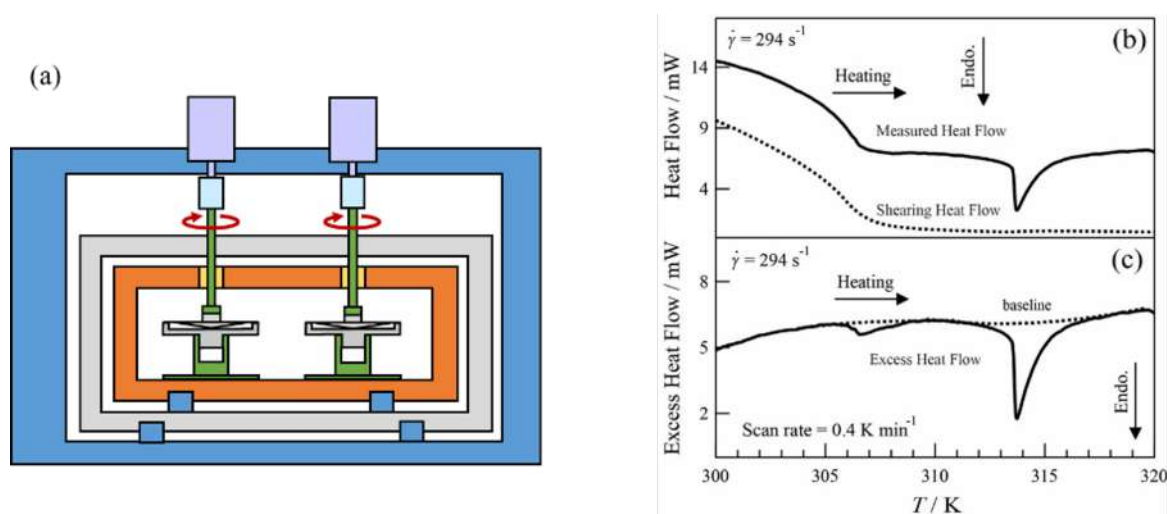


Figure 1: (a) Schematic of Shear-DSC. (b), (c) Results of Shear-DSC measurement for 8CB.

- [1] T. Yamamoto, H. Suzuki *et al.*, *Soft Matter*, 19 (2023) 1492-1498.
- [2] T. Yamamoto, H. Suzuki *et al.*, *Thermochim. Acta*, 730 (2023) 179629.

CONTRIBUTED TALK, TUE./10:05

Computational insights on dynamics of 1-butyl-3-methylimidazolium tetrafluoroborate ionic liquid with different water concentration

A. Pajzderska¹ and M. A. Gonzalez²¹*Faculty of Physics, A. Mickiewicz University, Poznań, Poland*²*Institut Laue-Langevin, 71 Avenue des Martyrs, CS 20156, 38042 Grenoble Cedex 9, France***email:** apajzder@amu.edu.pl

Ionic liquids (ILs) are well-known compounds consisting of organic cations and inorganic or organic anions with a melting point below 100 °C. Due to their physicochemical properties (negligible vapor pressure, high ionic conductivity, nonflammability, wide range of solubility, etc.), they are considered for use in a variety of applications, such as potential solvents for synthesis, sensors, fuel cells, and energy storage systems.

We present a molecular dynamics simulation study of 1-butyl-3-methylimidazolium tetrafluoroborate $[C_4mim][BF_4]$ with different water concentrations (up to 70%, for light and heavy water). This system is fully water-miscible, which makes it possible to study the influence of water on the structural and dynamical properties of ILs. In particular, we compare the pair distribution function and static structure factor with experimental diffraction data. We focus on the analysis of the dynamics of tetrafluoroborate anions, imidazolium cations, and water molecules by analyzing their diffusion coefficients. Additionally, comparing the neutron dynamic total structure factor with recent quasielastic neutron scattering research will provide insight into the dynamics of the imidazolium cation and better understand the origin of different water species detected experimentally [1]

[1] M. D. Ruiz-Martin *et al.*, J. Chem. Phys., 156 (2022) 084505

CONTRIBUTED TALK, TUE./10:20

Modification of the liquid-crystalline order in itraconazole using mechanical stress, temperature variation, and solvation

T. Lamrani¹, P. Jesionek^{2,3}, M. Tarnacka¹, B. Hachuła², D. Zakowiecki⁴, E. Ozimina-Kamińska³, K. Kamiński¹, and K. Jurkiewicz¹

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Liquid crystals (LCs) with molecular organisation between crystalline and amorphous states have gained significant attention in pharmaceutical research due to their properties [1]. These partially ordered systems can form two basic mesophase arrangements, i.e., nematic and smectic, through thermotropic or lyotropic transitions. The ability to modulate and control these transitions is crucial, as they significantly impact the physicochemical characteristics and performance of LC compounds in drug delivery applications.

This study investigates the structural properties of a famous small-molecular active pharmaceutical ingredient able to form LC phases – itraconazole. We demonstrate that, besides temperature variation and solvation, mechanical stress introduced by cryo-milling may also generate the liquid-crystalline transition in itraconazole. Moreover, by variation in the milling time and frequency, the nearest-neighbour order may be tuned, which affects the important properties from the pharmacy point of view, and physical stability and solubility.

By using X-ray diffraction and dielectric spectroscopy, we reveal that, compared to smectic itraconazole phase trapped in the glass via vitrification, the nematic phases obtained by cryo-milling are characterised by increased intermolecular distances and enhanced structural relaxation above the glass transition temperature. Moreover, we show that by selecting an appropriate solvent and its concentration, as well as by pressure densification and cooling rate, we are able to tune the degree of the smectic order in itraconazole.

This work provides valuable insights for formulating stable liquid crystalline phases of pharmaceuticals, thereby paving the way for improved drug delivery strategies.

Acknowledgements: The authors acknowledge financial support from the National Science Centre, grant number 2021/41/B/NZ7/01654

[1] C. L. Stevenson *et al.*, *J. Pharm. Sci.*, 94 (2005) 1861

SPECTROSCOPIC AND DIFFRACTION METHODS

Chair: Max Wolff

11:05	Serguei Molodtsov (Schenefeld, Germany) European XFEL: how does it work and fascinating applications	p. 13
11:40	Paweł Korecki (Kraków, Poland) Updates from SOLARIS national synchrotron radiation centre	p. 14
12:10	Cristian Svetina (Madrid, Spain) X-rays transient gratings at the european X-ray free electron laser	p. 15
12:40	Sebastião Antunes (Hamburg, German) Reconciliation of theoretical predictions and volume integrated experimental data in ultrafast X-ray science through calculation of effective fluence	p. 16
12:55	Sara El Houbbadi (Kraków, Poland) Revealing the molecular structure of copper phosphonate groups anchored inside SBA-15 silica channels: theoretical and experimental study	p. 17

KEYNOTE, TUE./11:05

European XFEL: how does it work and fascinating applications

S. Molodtsov¹

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The European X-ray Free Electron Laser (XFEL) is a new international research installation that is in operation in the Hamburg area in Germany. The facility generates new knowledge in almost all the technical and scientific disciplines that are shaping our daily life - including nanotechnology, medicine, pharmaceuticals, chemistry, materials science, power engineering and electronics. The ultra-high brilliance femtosecond X-ray flashes of coherent radiation are produced in a 3.4-kilometre long European XFEL facility. Most of it is housed in tunnels deep below ground. In its start-up configuration, the European XFEL comprises 3 self-amplified spontaneous emission (SASE) light sources – undulators operating in energy ranges 3 - 25 keV (SASE 1 and SASE 2) and 0.2 - 3 keV (SASE 3), respectively. The world-unique feature of this XFEL is the possibility to provide up to 27.000 ultra-short flashes (1 - 100 fs) that makes the facility particular suitable for time-resolved photoemission, (resonance) inelastic X-ray scattering, diffraction and imaging studies in the range of moderate and hard X-ray photons.

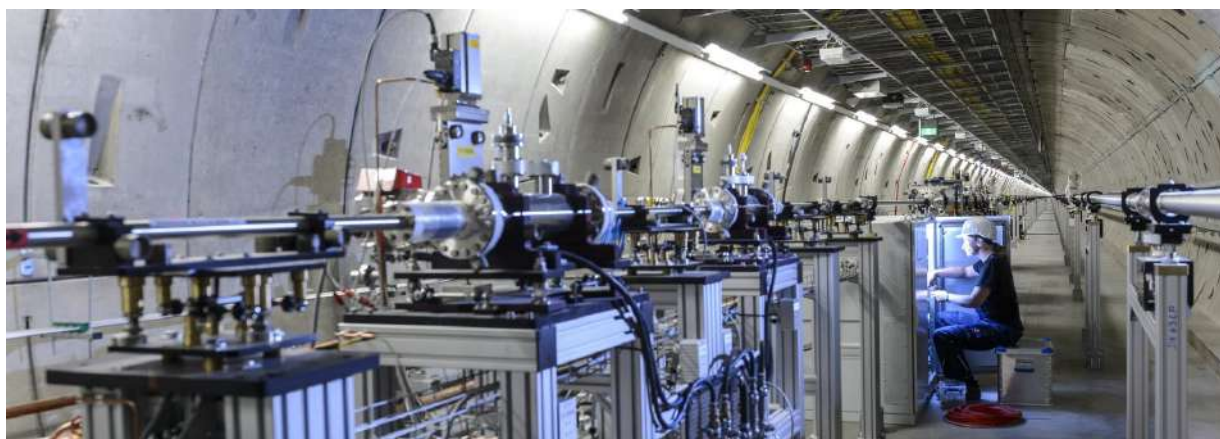


Figure 1: European XFEL beamline

In this lecture, basics of XFEL's operation as well as an overview of the European XFEL project will be provided and a review of various applications including time-resolved studies will be given.

INVITED TALK, TUE./11:40

Updates from SOLARIS national synchrotron radiation centre

P. Korecki

SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, Krakow, Poland

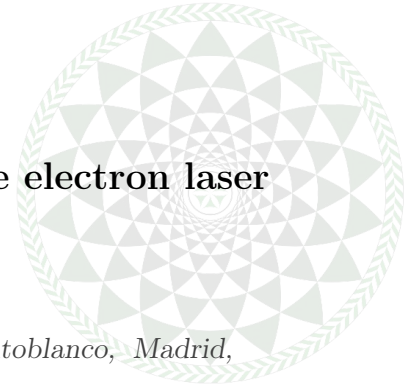


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The SOLARIS synchrotron in Krakow is a third-generation synchrotron radiation source operating in the medium electron energy range. The first synchrotron light in SOLARIS was observed in 2016, while the first user experiments were performed in 2018. SOLARIS is expanding its activities, constantly developing experimental beamlines and complementary infrastructure such as cryo-electron microscopes. Research opportunities offered by SOLARIS, the only synchrotron in Central-Eastern Europe, allow for conducting unique scientific projects in fundamental research and applied sciences. In the presentation, we will present the SOLARIS synchrotron project and available infrastructure, provide practical information on access to the infrastructure, and show examples of the research results obtained at the Centre by the Users.

Acknowledgements: We acknowledge the Polish Ministry and Higher Education project Support for research and development with the use of the research infrastructure of the National Synchrotron Radiation Centre SOLARIS' under contract nr 1/SOL/2021/2.

INVITED TALK, TUE./12:10



X-rays transient gratings at the european X-ray free electron laser

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Transient Grating (TG) spectroscopy, a special case of wave-mixing [1], employs two crossed laser beams interacting at the sample generating an interference pattern while a third time-delayed probe beam is used to monitor the time evolution of the induced dynamics in the sample revealing information on transport and diffusion processes and quasi-particle dynamics.[2] Optical wavelengths inherently limit the reachable spatial and temporal resolutions while extension to higher photon energies - i.e. extreme ultraviolet and X-rays - allows to potentially reach nanometer and atto-femtosecond scales adding element and chemical specificity being able to access to K, L and M resonances.[3] In the last years a large international community has formed to study extension of TG in the X-rays.[4, 5] In the talk I will describe and advances and status of the Long Term Proposal “Dynamics of nanoscale phenomena in solids and liquids studied with X-ray Transient Gratings at European XFEL” [6] showing the latest results and look at the future activities. I will conclude introducing the COST Action NEXT for the development and application of nonlinear wave-mixing methods in the extreme ultraviolet and X-rays.[7]

[1] R.L. Sutherland, Handbook of Nonlinear Optics, 2nd Edition, CRC Press (2003)

[2] H.J. Eichler *et al.*, Laser-Induced Dynamic Gratings, Springer (1986)

[3] M. Chergui *et al.*, Nat. Rev. Phys., 5 (2023) 578

[4] C. Svetina *et al.*, Opt. Lett., 44 (2019) 574

[5] J. R. Rouxel *et al.*, Nat. Photon., 15 (2021) 499

[6] <https://www.nanociencia.imdea.org/home-en/news/item/mixing-x-rays-the-future-of-ultrafast-science>

[7] <https://www.cost.eu/actions/CA22148/>

CONTRIBUTED TALK, TUE./12:40

Reconciliation of theoretical predictions and volume integrated experimental data in ultrafast X-ray science through calculation of effective fluence

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In pump-probe experiments within ultrafast X-ray science, an X-ray pump pulse deposits energy in a solid sample with a non-uniform spatial distribution. This results in different parts of the sample being exposed to different pulse fluences. The following X-ray probe pulse then measures a volume integrated average of contributions from the differently irradiated regions of the sample.[1]

Starkly contrasting with the experimental scheme, computational simulations of the X-ray irradiated samples typically use periodic boundary conditions which implies an assumption of a uniform X-ray irradiation.[2] Obtaining a prediction on a volume integrated observable requires a significant computational effort, as it is necessary to perform multiple simulations for the different exposure conditions and then perform their volume integration.

Here we propose an analytical scheme to calculate an effective fluence such that the observable of interest calculated with the effective fluence would “mimic” the volume-integrated observable. This calculation is based on how the observable in question depends on X-ray fluence.

We demonstrate the effectiveness of the method with XTANT simulations [2] performed for silicon crystal pumped with 50 eV photons. We obtain volume-integrated time series for average atomic displacements and intensities of different Bragg diffraction peaks. After applying a dedicated analytical scheme, a comparison of volume integrated results with the effective fluence results is made, with very satisfactory results.

[1] V. Tkachenko *et al.*, Appl. Sci., 11 (2021) 5157

[2] N. Medvedev *et al.*, New. J. Phys., 15 (2013) 015016

CONTRIBUTED TALK, TUE./12:55

Revealing the molecular structure of copper phosphonate groups anchored inside SBA-15 silica channels: theoretical and experimental study

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This work used X-ray absorption spectroscopy to examine copper sites' geometric environment and valence states in mesoporous silica containing copper phosphonate. The main goal was to verify the actual geometry of the copper functional groups. Quantitative analysis of the EXAFS data was challenging due to the amorphous nature of the sample, which prevented the fulfilment of the Nyquist criterion in Artemis software used to fit the EXAFS equation.

To address these challenges, we employed numerical methods to analyse the XANES spectrum, which provides information about the oxidation state and local electronic structure of the absorbing atom. Thousands of theoretical spectra were calculated using geometrically optimized copper molecular groups with various structural characteristics. By employing linear combination fitting to the experimental spectrum, we identified a combination of models: 62% BA06, 27% BA09, and 21% BA05. These models represent slightly different configurations of a copper atom intricately coordinated by two phosphonate groups, forming a pseudo-bi-trigonal pyramid environment composed of oxygen atoms [1].

These findings are critical to understanding the antibacterial and nonlinear optical (NLO) properties of the hybrid material [2, 3].

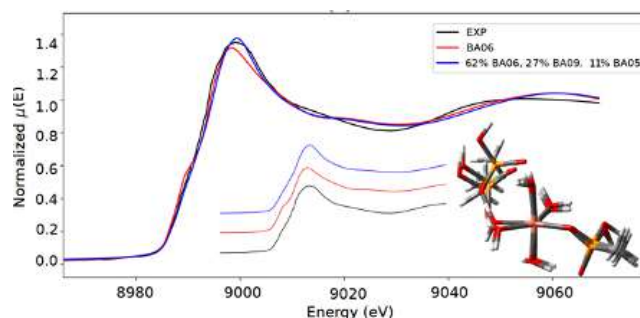


Figure 1: The experimental XANES spectrum (EXP) and the closest simulated XANES spectra

Acknowledgements: Financial support for this investigation has been provided by the National Centre of Science (2020/37/B/ST8/03637, and 2021/43/D/ST8/00737).

- [1] S. El Houbbadi *et al.*, Appl. Surf. Sci., 669 (2024) 160425
- [2] M. Laskowska *et al.*, Nanoscale, 33 (2017) 12110
- [3] L. Laskowski *et al.*, J. Nanomater., 2017. (2017) 1287698

MULTIFUNCTIONAL MATERIALS

Chair: Silvina Cerveny

- 14:30 **Neven Žitomir Barišič** (Wien, Austria) p. 19
High- T_c cuprates – story of two electronic subsystems
- 15:05 **Yuki Utsumi Boucher** (Zagreb, Croatia) p. 20
Electronic and crystal structures of EuTGe_3 (T : transition metal) under extreme conditions
- 15:35 **Alessandro Surrente** (Wrocław, Poland) p. 21
Spin polarization dynamics in WSe_2 monolayer and in $\text{WSe}_2/\text{BAPbI}_4$ heterostructure
- 16:05 **Priyanka Reddy** (Zagreb, Croatia) p. 22
Murunskite: a bridge between cuprates and pnictides
- 16:20 **Serena Nasrallah** (Fribourg, Switzerland) p. 23
 EuCd_2X_2 : semimetal illusion versus semiconductor reality

Chair: Mário Rosado

- 17:05 **Petar Popčević** (Zagreb, Croatia) p. 24
Electronic transport in magnetically intercalated 2H-NbS_2 : what can we learn from the electronic structure
- 17:35 **Wojciech Tabiś** (Kraków, Poland) p. 25
Correlation between magnetism and the Verwey transition in magnetite

KEYNOTE, TUE./14:30

High- T_c cuprates – story of two electronic subsystems

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Materials science and high technologies are the driving force of any advanced society. The phenomenon of high-temperature superconductivity, found in cuprates, is of undisputable technological importance. It also presents one of the most exciting, thoroughly investigated yet still unresolved problems in physics. A major difficulty in understanding high- T_c systems lies in the complexity of the materials and phase diagram, where the delicate balance between material specific properties, disorder and the number of electronic phases superimpose makes it hard to identify the leading interactions. Despite the complexity, we have identified a series of surprisingly simple and universal behaviors [1–7]. Based on them we show that the phenomenology of cuprates across the phase diagram is fully captured by the simple charge conservation relation:

$$1 + p = n_{\text{loc}} + n_{\text{eff}}.$$

Here, p is the doping while n_{eff} is the carrier density and n_{loc} is the density of localized charge within a CuO_2 plaquette. The corresponding superfluid density is related to both components:

$$\rho_S = n_{\text{eff}} \cdot (O_S n_{\text{loc}}),$$

where all terms can be experimentally determined directly. The charge n_{loc} is responsible for all the strangeness of these compounds, which includes the pseudogap phenomenon and the superconducting glue [7–9]. The compound-dependent constant, O_S , is fine-tuned by the local crystal structure. It arises from the $p \sim d \sim p$ fluctuation by the Cu-localized holes visiting the neighboring planar-oxygen atoms and can be determined from NMR [9].

- [1] N. Barišič *et al.*, *New J. Phys.* 21, (2019), 113007 (see also arXiv:1507.07885 (2015))
- [2] Y. Li *et al.*, *Sci. Adv.* 5, (2019), eaap7349
- [3] N. Barišič *et al.*, *Proc. Natl. Acad. Sci. U.S.A.* 110, (2013), 12235
- [4] S. I. Mirzaei *et al.*, *Proc. Natl. Acad. Sci. U.S.A.* 110, (2013), 5774
- [5] M. K. Chan *et al.*, *Phys. Rev. Lett.* 113, (2014), 177005
- [6] P. Popčević *et al.*, *npj Quantum Mater.* 3, (2018), 42
- [7] C. M. N. Kumar *et al.*, *Phys. Rev. B* 107, (2023), 144515
- [8] D. Pelc *et al.*, *Sci. Adv.* 5, (2019), eaau4538
- [9] N. Barišič & D. K. Sunko, *J Supercond. Nov. Magn.* 35, (2022), 1781

INVITED TALK, TUE./15:05

Electronic and crystal structures of $\text{Eu}T\text{Ge}_3$ (T : transition metal) under extreme conditions

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⁷*Department of Earth Sciences, Department of Physics and Astronomy, University of Western Ontario, N6A-5B7, Canada.*

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Non-centrosymmetric $\text{Eu}T\text{Ge}_3$ (BaNiSn_3 -type structure, $I4mm$) has been attracting considerable attention due to complex magnetic structures [1, 2]. The magnetism arises from Eu^{2+} ($4f^7$, $J = 7/2$) ions while transition metal is non-magnetic. The moments' ordering direction varies depending on transition metal, temperature, and external magnetic field. Although temperature- and field-induced magnetic phase transitions have been reported among the $\text{Eu}T\text{Ge}_3$ series, their electronic and crystal structures under pressure remain to be studied. Since the Eu oxidation state is directly related to the magnetic behavior and provides complementary information to understand the pressure phase diagram, we studied the pressure evolution of the Eu oxidation state of $\text{Eu}T\text{Ge}_3$ ($T=\text{Co, Rh, Ir}$) by near-edge x-ray absorption spectroscopy (XAS). The Eu L_3 near-edge XAS spectra showed an increase (decrease) of Eu^{3+} (Eu^{2+}) peak intensity by applying pressure. In all three compounds, the average oxidation state of Eu strongly deviated from the integer under pressure showing a valence fluctuation behavior. We also performed powder x-ray diffraction in $\text{Eu}T\text{Ge}_3$ ($T=\text{Co, Rh, Ir}$) under pressure to study pressure-induced structural evolution concerning changes in the Eu oxidation state. Our results showed a smooth contraction of the lattice volume without symmetry changes by increasing pressure, though an anisotropic compressibility between the a - and c -axis was revealed [3].

Acknowledgements: The Croatian Science Foundation has partly supported this work under the project numbers UIP 2019-04-2154, IP 2020-02-9666, and by the project Cryogenic Centre at the Institute of Physics –KaCIF co-financed by the Croatian Government and the European Union through the European Regional Development Fund-Competitiveness and Cohesion Operational Programme (Grant No. KK.01.1.1.02.0012).

- [1] O. Bednarchuk *et al.*, J. Alloys Comp., 622 (2015) 432-439.
- [2] D. Singh *et al.*, Nat. Commun., 14 (2023) 8050.
- [3] N. S. Dhimi *et al.*, Phys. Rev. B, 107 (2023) 155119.

INVITED TALK, TUE./15:35

Spin polarization dynamics in WSe₂ monolayer and in WSe₂/BAPbI₄ heterostructure

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In the first part of this talk, I will show how it is possible to optically inject an exciton spin polarization in a monolayer WSe₂ with a helicity opposite with respect to that of the excitation laser. This result, shown as negative degree of circular polarization in the photoluminescence (PL) and PL excitation (PLE) of Fig. 1(a,b), is rationalized by accounting for a Dexter-type intervalley scattering mechanism [1].

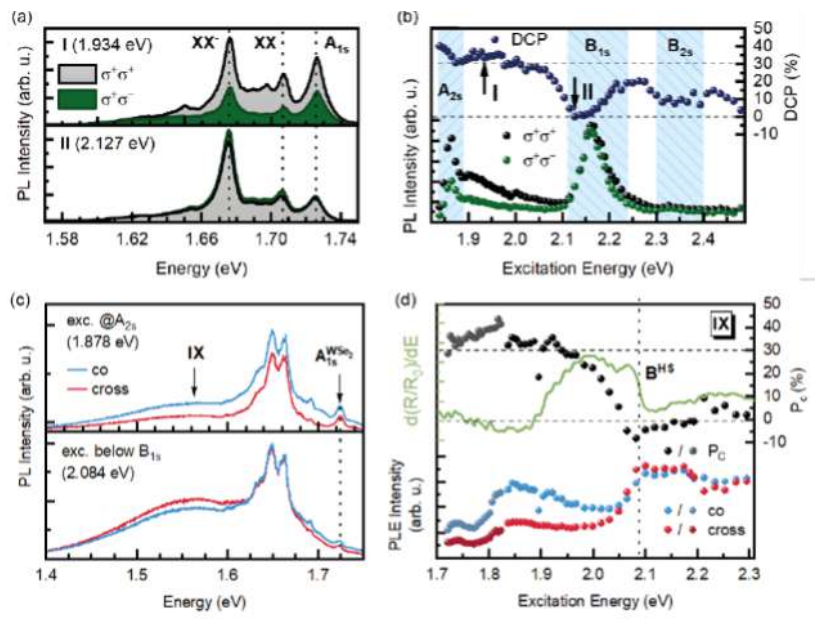


Figure 1: PL spectrum of monolayer WSe₂ with detection of the light co-polarized ($\sigma^+\sigma^+$) and cross-polarized ($\sigma^+\sigma^-$) to excitation. (b) Excitation energy dependent PL intensity of the co- and cross-polarized emission and calculated degree of circular polarization (DCP). (c) PL spectrum resolved in circular polarization of a WSe₂/BAPbI₄ heterostructure. (d) Excitation energy dependence of the intensity and DCP of the interlayer exciton (IX) in this heterostructure.

In the remaining part of the talk, I will focus on the optical properties of the (spatially indirect) interlayer exciton formed in a WSe₂/BAPbI₄ heterostructure. Our pump-probe measurements demonstrate that this complex is formed upon ultrafast hole transfer from WSe₂ to the BAPbI₄ perovskite compound. Polarization resolved PL and PLE measurements shown in Fig. 1(c,d) demonstrate that this species exhibits circular dichroism when the luminescence is excited by circularly polarization light. This suggests that the charge transfer preserves the spin optically injected in WSe₂, which is a very convenient manner of “sensitizing” the circular dichroism in a two-dimensional perovskite material without making use of cumbersome chiral organic spacers.

[1] J. Jasinski, *et al.*, 2D Materials 11 (2024) 025007.[2] J. Jasinski, *et al.*, in preparation.

CONTRIBUTED TALK, TUE./16:05

Murunskite: a bridge between cuprates and pnictides

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Despite exceptional scientific efforts over several decades, there is almost no universal agreement about the superconducting state of cuprate compounds. A constructive way to improve understanding would be to synthesize and investigate a new system, which displays superior chemical flexibility and tunability of the valence of the transition metal ions. One could then manipulate its various electronic, metallic, and mechanical properties. We study murunskite, which interpolates between cuprates and pnictides [1]. This presentation will report the successful growth and characterisation of the first-ever high-quality Murunskite single crystals. These crystals show semiconductors like the parent compounds of cuprates, yet isostructural to the metallic iron-pnictides. Moreover, like both families, it has an antiferromagnetic response with an ordered phase below 100 K. Spectroscopy (XPS) and Density Functional Theory (DFT) calculations concur that the sulfur 3p orbitals are partially open, making them accessible for charge manipulation, which is a prerequisite for superconductivity in analogous layered structures. Furthermore, DFT indicates that the valence band is more cuprate-like, while the conduction band is more pnictide-like. We also managed to substitute Fe with Co in the parent compound, leading to superconductivity in this family for the first time.

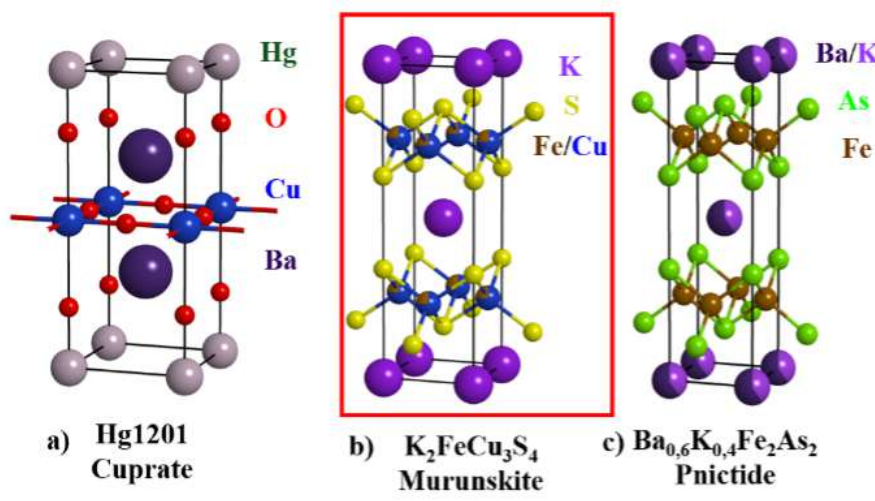


Figure 1: Comparison of murunskite structure b) with a cuprate a) and pnictide c)

[1] D. Tolj *et al.*, Appl. Mater. Today, 24 (2021) 101096

CONTRIBUTED TALK, TUE./16:20

EuCd₂X₂: semimetal illusion versus semiconductor reality

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The search for intrinsic magnetic topological materials has captured the interest of numerous scientists in recent years due to their potential spintronic application. EuCd₂X₂ ($X = \text{Sb, As, P}$) family was predicted by Density Functional Theory (DFT) to be a topological, Weyl semimetal. [1, 2] This claim was further supported by transport measurements and Angle-Resolved Photoemission Spectroscopy (ARPES), which exhibited metallic-like resistivity and the conical shape of the valence band, respectively. [3, 4]

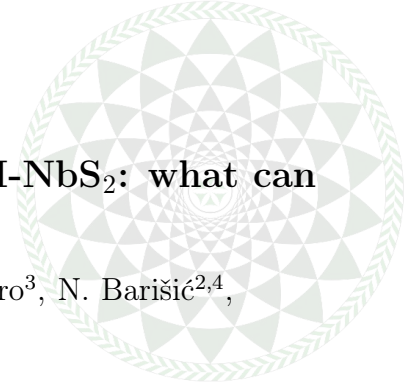
However, our recent infrared- and magneto-optics measurements revealed that EuCd₂X₂ is a magnetic semiconductor rather than a topological Weyl semimetal. We obtained energy gaps of 0.5 eV, 0.77 eV, and 1.2 eV for $X = \text{Sb, As, and P}$, respectively.[5, 6] These band gaps are notably influenced by the application of a magnetic field, undergoing redshifts of 45 meV, 125 meV, and 150 meV, respectively. Despite these shifts, magneto-optics shows that the band gaps do not close even under the application of a high field of 35T, indicating that the compounds remain semiconductors and thus excluding a magnetic Weyl semimetal scenario.

Additionally, ARPES and pump-probe ARPES on EuCd₂As₂ confirmed the band gap of 0.7 eV. The resistivity measurements revealed activation behavior for EuCd₂As₂ and EuCd₂P₂, while EuCd₂Sb₂ exhibited metallic-like resistivity, implying that the system is doped.

In conclusion, our study provides valuable insights into the effects of element substitution on the electronic band structure of EuCd₂X₂ semiconductors.

- [1] S. Hua *et al.*, Phys. Rev. B, 98 (2018) 201116
- [2] H. Su *et al.*, APL Materials, 8 (2020) 011109
- [3] Y. Shi *et al.*, Phys. Rev. B, 109 (2024) 125202
- [4] J. Ma *et al.*, Adv. Materials, 32 (2020) 1907565
- [5] D. Santos-Cottin *et al.*, Phys. Rev. Lett., 132 (2023) 186704
- [6] S. Nasrallah *et al.*, unpublished

INVITED TALK, TUE./17:05



Electronic transport in magnetically intercalated 2H-NbS₂: what can we learn from the electronic structure

P. Popčević¹, Y. Utsumi Boucher¹, G. Pransu¹, I. Batistić², L. Forro³, N. Barišić^{2,4}, and E. Tutiš¹

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Transition-metal dichalcogenides (TMDs) are quasi-2D compounds with a layered structure that allows for intercalation by various atomic and molecular species. Intercalating transition metal ions introduces magnetic sublayers with diverse interactions, leading to complex magnetic and potentially topological ground states. This makes them promising candidates for new electronic devices and applications.

In this study, we present Co_{1/3}NbS₂ and Ni_{1/3}NbS₂, both of which order antiferromagnetically. Despite having the same crystal structure, their magnetic and electronic transport properties reveal differences between the roles that Co and Ni ions play in the structure. To understand these differences, we explore the electronic structure of two compounds using angle-resolved photoemission spectroscopy (ARPES), ab-initio electronic structure calculations, and modeling [1–3].

Our findings show that intercalated ions dominate the interlayer coupling, highlighting the role of hybridization between intercalated orbitals and conducting layers. In Co_{1/3}NbS₂, we propose a “spin-valve” mechanism where the intercalated Co ions act as spin-selective electrical transport bridges between the host layers. In contrast, Ni ions in Ni_{1/3}NbS₂ effectively reduce electronic interlayer transport.

[1] P. Popčević *et al.*, Phys. Rev. B, 105 (2022) 155114.

[2] P. Popčević *et al.*, Phys. Rev. B, 107 (2023) 235149.

[3] Y. Utsumi Boucher *et al.*, Phys. Rev. B, 109 (2024) 085135.

INVITED TALK, TUE./17:35

Correlation between magnetism and the Verwey transition in magnetite

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Seeking to unravel the enigmatic Verwey transition and its interplay with magnetism, we conducted comprehensive measurements on the temperature-dependent electrical resistivity and magnetic moment of stoichiometric and doped-magnetite single crystals at temperatures reaching 1000 K. These investigations allowed us to identify the Curie temperature T_C , and other characteristic temperatures of the electrical resistivity. Remarkably, we identified correlations between these temperatures and the Verwey temperature T_V indicating that the electrical transport properties and the mechanism of the Verwey transition are closely related to the magnetic properties. During the presentation, this connection will be discussed in the context of the most recent work on magnetite.

Acknowledgements: The work was supported by the National Science Centre, Poland, Grant No. 2021/41/B/ST3/03454, and the “Excellence Initiative-Research University” program for AGH University of Krakow.



FLASH TALKS

Chair: Mário Rosado

- Liliia Kotvytska** (Košice, Slovakia)
18:05 Analysis of the physical properties of the ZIF-67 and its diamagnetic analogue ZIF-8 p. 27
- Anna Janowska** (Chorzów, Poland)
18:09 Molecular dynamics simulations of the structure of amorphous pharmaceutical – probucol p. 28
- Sebastian Lalik** (Kraków, Poland)
18:13 An effect of small Au nanoparticle concentrations onto chosen properties in liquid crystal exhibits SmC_A^* phase p. 29
- Arkadiusz Zarzycki** (Kraków, Poland)
18:17 Unusual phase transformation kinetics in FePd thin films – inter-mediated phases and its magnetic properties p. 30
- Marcin Perzanowski** (Kraków, Poland)
18:21 Asymmetric magnetization reversal tailored by different oxidation procedures in Co/CoO exchange-biased thin films p. 31
- Katarzyna Chat** (Kraków, Poland)
18:25 The interplay between thermal history and pressure and volume changes on the non-equilibrium behavior of polymers p. 32
- Mohammad S. Shakeri** (Kraków, Poland)
18:29 Pulsed laser induced solvent-nanoparticle chemo-physical interaction; an effective approach toward creation of submicron heterostructures p. 33
- Aleksandra Deptuch** (Kraków, Poland)
18:33 Liquid crystalline glassformer forming hexatic smectic X_A^* glass – DFT calculations for interpretation of X-ray diffraction and IR spectroscopy data p. 34
- Anna Drzewicz** (Kraków, Poland)
18:37 Self-assembly behavior of difluoroterphenyl derivatives differing with the linking bridge type p. 35
- Marcin Piwowarczyk** (Kraków, Poland)
18:41 Investigation of phase behaviour and selective light reflection in mixtures with azo compounds p. 36

FLASH TALK, TUE./18:05

Analysis of the physical properties of the ZIF-67 and its diamagnetic analogue ZIF-8

L. Kotvytska¹, R. Tarasenko¹, O. Lyutakov², M. Erzina², M. Orendáč¹, and A. Orendáčová¹

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Zeolitic imidazolate framework (ZIF) materials represent metal–organic frameworks with three-dimensional porous structure formed by metal ions linked via imidazole linkers. This work is devoted to the study of $[\text{Co}(\text{mIm})_2\alpha]$, abbreviated as ZIF-67 and its diamagnetic analogue $[\text{Zn}(\text{mIm})_2\alpha]$ known as ZIF-8 ($\text{HmIm} = 2\text{-methylimidazole} = \text{C}_4\text{H}_6\text{N}_2$). The rapid synthesis in water produced nanocrystallites. XRD, infrared and Raman measurements confirmed that both compounds have identical crystal structure and vibration spectra with the only difference that Co atoms in ZIF-67 occupy the positions of Zn in ZIF-8.

The heat capacity of the powder samples was measured from 0.4 to 300 K in zero magnetic field. Magnetic specific heat of ZIF-67 was obtained by subtraction of ZIF-8 specific heat which can be treated as lattice contribution. The magnetic contribution C_{mag} is characterized by a round maximum at 11 K, typical for low-dimensional systems. Corresponding magnetic entropy agrees with the prediction for spin 3/2. The application of magnetic field had negligible effect on the round maximum. The magnetic susceptibility in 10 mT shows bifurcation of field cooling (FC) and zero field cooling (ZFC) data at 14 K but in 100 mT the splitting shifts to 5 K and finally it disappears completely in fields above 1 T. The application of Curie–Weiss law provides $g = 2.2$ and $\theta = -44$ K, reflecting moderate antiferromagnetic interactions. The isothermal magnetization $M(B)$ of ZIF-67 was measured at 0.46 K. At fields up to 1T, the $M(B)$ deviates from the linear dependence, which corresponds with the appearance of bifurcation of ZFC and FC data below 1 T. The character of magnetism in ZIF-67 is discussed.

Acknowledgements: The work was supported by the projects APVV-22-0172, VEGA 1/0132/22 and VVGS-2023-3040.

FLASH TALK, TUE./18:09

Molecular dynamics simulations of the structure of amorphous pharmaceutical – probucol

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Amorphous-like pharmaceuticals have recently gained a lot of interest since they exhibit better solubility and bio-availability compared to their crystalline counterparts commonly used in tablet forms. Usually, such amorphous forms of active pharmaceutical ingredients (APIs) are produced by vitrification of melt. However, the variation in the melting temperature, cooling rate as well as applying mechanical milling or compression may affect their atomic-scale structure and related properties important from the application point of view [1, 2]. Therefore, understanding of basic correlations between the preparation process, structure, and properties is a prerequisite for further development of the amorphous pharmaceutical technology and their commercialization.

Due to very limited possibility of interpretation of subtle differences in the structure of various amorphous-like phases using standard characterization methods such as X-ray diffraction, usage of computer simulations is highly desired for verification of experimental data and obtaining of structural features difficult to extract based on solely of experimental data.

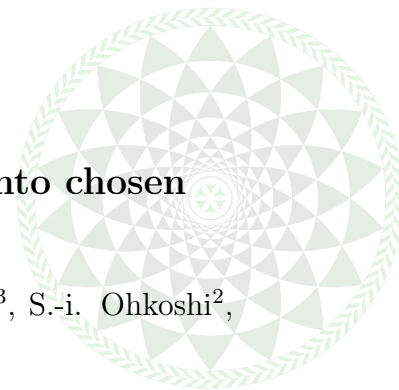
Here, Gromacs software was used to perform molecular dynamics simulations of the system of probucol API – is an anti-hyperlipidemic drug, at various temperature and pressure conditions in order to understand the changes into the intra- and inter-molecular structure induced by cooling and compression. The analysis of the total and partial structure factors, radial distribution functions, hydrogen bonds and molecular conformations allowed us to recognize differences in the structure between glasses produced by standard vitrification and the so-called “pressure-densification” method.

Acknowledgements: The authors acknowledge financial support from the National Science Centre, grant number 2021/41/B/NZ7/01654

[1] D. Heczko *et al.*, *J. Mol. Liq.*, 351 (2022) 118666

[2] M. Rams-Baron *et al.*, *Appl. Phys. Lett.*, 111 (2017) 121902

FLASH TALK, TUE./18:13



An effect of small Au nanoparticle concentrations onto chosen properties in liquid crystal exhibits SmC_A^* phase

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A very simple and cheap way to obtain new liquid crystalline materials is to introduce nanoparticles (NPs) into the liquid crystal matrix. In our studies we used well-known liquid crystal (S)-MHPOBC as a matrix and Au nanoparticles (0.2 and 0.5wt.%) as dopant to check how the nanomaterial affects the properties of the matrix [1]. (S)-MHPOBC exhibits rich polymorphism and antiferroelectric phase SmC_A^* in a wide temperature range, therefore the research focused on the SmC_A^* phase. It was found that NPs do not influence liquid crystalline phases, however they are responsible for new crystal phases at concentration 0.5wt.%. The molecular reorientation time τ depends on the NPs concentration, which is related to the modified local electric field very close to the nanoparticle surface. In turn, the tilt angle θ is bigger only for concentration 0.5 wt.% Au NPs. The spontaneous polarization P_S is higher for both concentration which is associated to localized surface plasmonic resonance. The mentioned resonance is responsible for the induction of an electric dipole moment in the nanoparticle in the visible range, which in turn generates a strong electric field in its vicinity. The induced additional dipole moment contributes to the macroscopic polarization and the organic molecules surrounding the NPs experience a stronger electric field. The smectic layer distance D as well as the correlation length ξ is not affected by Au NPs. In the same time, the helical pitch p is increased in comparison to pure matrix and it decreases with decreasing temperature. Additionally, the influence of Au NPs on localization of absorption bands, electric permittivity, specific electric conductivity and relaxation processes will be presented.

[1] S. Lalik *et al.*, *Molecules*, 27 (2022) 3663

FLASH TALK, TUE./18:17



Unusual phase transformation kinetics in FePd thin films – intermediated phases and its magnetic properties

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In this study, we investigate the phase transformation process between Fe/Pd multilayer and L1₀ FePd alloy. The transformation is studied at different stages of post-deposition annealing to track the progress of chemical ordering and phase transformation. For that purpose, we combined SEM, XRD and Mossbauer spectroscopy techniques. It allowed to identify an unusual way of transformation through two parallel and competitive paths. The first one includes the stoichiometric route of A1 and A6 phases, and the second off-stoichiometric route with L1₂ and L1' phases. The process ends with the formation of the L1₀ phase. We found that one of the most important factors determining the type of phase transformation is solid state dewetting. When the dewetting progresses rapidly the change in the kinetic growth is observed from a low-dimensional to a three-dimensional growth mechanism that primarily affects the L1₀ phase formation [1].

Parallel to structural research, we study the changes in magnetism properties with the evolution of film morphology and phase composition. We found that the major changes are observed when the dewetting progresses and the film loses its continuity. Then the fast growth of the L1₀ phase happens influencing the magnetization reversal mechanism and yielding the magnetic spring-like behavior [2]. Since the solid state dewetting process influences the type of phase transformation and intermediated phases contribution, it creates new opportunities for using this phenomenon to tailor the magnetic properties of thin alloy films.

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[2] A. Zarzycki *et al.*, Materials, 16 (2023) 16

FLASH TALK, TUE./18:21

Asymmetric magnetization reversal tailored by different oxidation procedures in Co/CoO exchange-biased thin films

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The exchange bias effect is a magnetic phenomenon associated with a unidirectional exchange anisotropy which appears at the interface between a ferromagnet and an antiferromagnet. Due to this coupling, the magnetization reversal in one field sweeping direction is more energetically demanding than in the other which leads to the shift of a magnetic hysteresis loop from the zero position known as the bias field H_{ex} . The exchange bias effect is sensitive to the condition of the interface between a ferromagnet and an antiferromagnet. Especially, its magnitude is dependent on the roughness of layers, intermixing of constituent materials, and structural order at the interface.

In this work, we report on the asymmetric magnetization reversal for the model CoO/Co exchange-biased system. The antiferromagnetic CoO layer was prepared in three different ways – natural oxidation in ambient conditions, oxidation in vacuum in partial oxygen pressure, and by plasma treatment. We focus on changes in magnetic properties induced by various procedures and combine them the condition of the antiferromagnetic-ferromagnetic interface studied by chemical depth profiling. The reversal along the upper hysteresis branch shows the wall motion while the switching along in opposite field direction indicates an influence of the coherent magnetization rotation. In all cases the hysteresis loops are asymmetrical and the asymmetry is dependent on the temperature and on the type of procedure used to obtain CoO layer (see Figure 1).

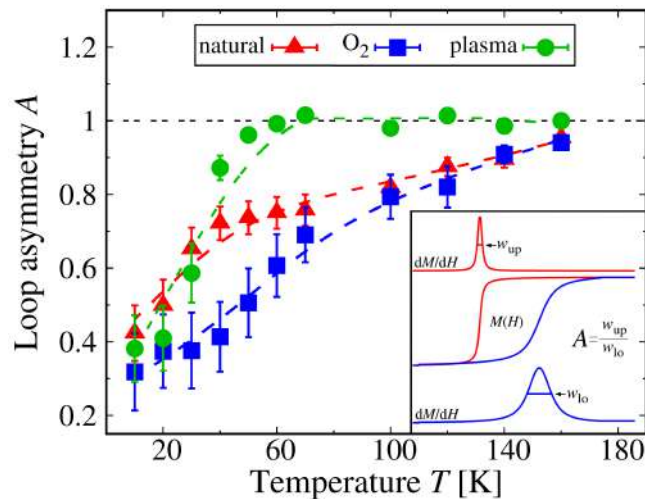


Figure 1: Magnetic hysteresis loop asymmetry parameter A calculated from the dM/dH switching field distributions measured for the natural, O_2 , and plasma samples. Dashed lines are a guide for the eye. The inset schematically shows the way the A parameter was determined.

Acknowledgements: The research was supported by the DAAD grants PPP-PL 57214850 and co-financed by the Polish National Agency for Academic Exchange, project BPN/BDE/2022/1/00005/U/00001. The HR-RBS measurements were performed in Ion Beam Center HZDR within the proposal 16000782-ST.

FLASH TALK, TUE./18:25

The interplay between thermal history and pressure and volume changes on the non-equilibrium behavior of polymers

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Literature data indicate that the various deviations from bulk behavior observed for polymers under nanoconfinement exhibit out-of-equilibrium features and can be eliminated through prolonged annealing. The time needed to recover the equilibrium state primarily depends on factors such as temperature, pore size, and the polymer's chain length [1–3]. In this presentation, we will discuss the influence of pressure and volume changes on the non-equilibrium glassy dynamics of poly(phenylmethyl siloxane) (PMPS 2.5k) confined within AAO nanopores. To explore this, we have conducted time-dependent measurements at the annealing temperature, following intermediate temperature jumps from higher (“down jump”) or lower (“up jump”) temperatures. Figure 1 illustrates the segmental relaxation times for PMPS 2.5k confined in 60 nm nanopores at the initial and final stages of annealing after up and down jumps. Our findings indicate that pore size, equilibration temperature, and depth jumps significantly influence the time required for the confined polymer to recover the segmental relaxation of the bulk sample. We have also shown that volume and pressure changes are closely linked with the equilibration process. After the down jump, the polymer needs to eliminate excess free volume to regain its bulk properties. Conversely, under up-jump conditions, the system gains volume during the annealing process, accompanied by corresponding pressure changes. Our study provides new arguments that the equilibration kinetics under nanopore-containment is related to volume and pressure changes.

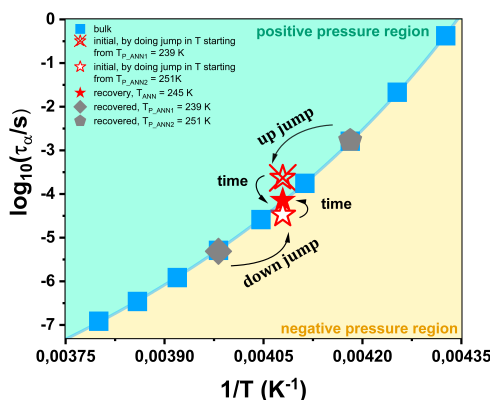


Figure 1: The segmental relaxation time vs inverse of temperature for PMPS 2.5k in bulk and confined in 60 nm nanopores. Data for confined samples were recorded under up- and down-jump conditions in the annealing temperature $T_{ANN} = 245$ K.

Acknowledgements: K. Chat is grateful for the financial support from the National Science Centre, Poland within the Project SONATINA 7 (dec. no. 2023/48/C/ST3/00179).

- [1] K. Adrjanowicz *et al.*, Phys. Rev. Lett., 122 (2019) 176101
- [2] P. Kardas *et al.*, J. Phys. Chem. B, 126 (2022) 5570
- [3] K. Chat *et al.*, J. Phys. Chem. C, 124 (2020) 22321

FLASH TALK, TUE./18:29

Pulsed laser induced solvent-nanoparticle chemo-physical interaction; an effective approach toward creation of submicron heterostructures

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Creating heterostructures has been a brilliant solution to address the increasing need for innovative materials in high-tech applications. Heterostructures possess distinct attributes that render them highly promising for the development of sustainable and environmentally friendly energy systems with a diverse range of applications across multiple fields, such as catalysis, energy storage, and solar energy harvesting. In this study, we aim to investigate a promising and innovative approach for producing heterostructures involving the use of pulsed laser irradiation on suspended nanoparticles. Our main focus lies in understanding the chemo-physical interactions that occur at the interface between the solvent and the nanoparticles when they are adjusted to the laser pulses. When the nanoparticles are exposed to the laser pulses, they absorb the energy from the pulses, causing the solvent molecules in contact with them to gain kinetic energy. This increase in energy is sufficient for the solvent molecules to dissociate and diffuse into the molten nanoparticle, leading to the formation of different phases [1]. The formation process involves both physical phase transitions and chemical oxidation/reduction reactions, which are highly influenced by the chemical environment and temperature of the reaction [2]. These variables were adjusted accordingly based on the suspension and laser parameters to achieve the desired heterostructures. An example of the formation of copper quantum dot on the surface of Fe_3O_4 using laser irradiation has been illustrated in Figure 1a. The particle growth mechanism is also depicted schematically in Figure 1b. Further exploration of the process by which phases were created is being studied through the application of atomistic modeling techniques. In this study, density functional theory (DFT) calculations were employed to determine the reactive bond force fields. These force fields are subsequently utilized to investigate the breaking and formation of bonds in the respective systems, employing molecular dynamics (MD) simulations.

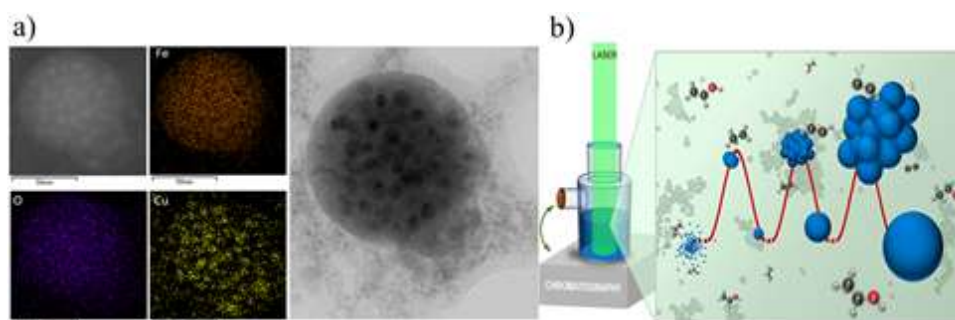


Figure 1: (a) Formation of copper quantum dot on magnetite nanoparticles, and (b) schematic of growth mechanism during pulsed laser irradiation of suspended nanoparticles.

Acknowledgements: This work is supported by the Polish National Science Center under programs No. 2018/31/B/ST8/03043 and 2022/06/X/ST3/01743. The calculations were also performed in the Prometheus Cluster, Cyfronet, under grant number PLG/2022/015573. We thank the Polish National Synchrotron Center (SOLARIS) and Elettra Synchrotron, Trieste, Italy for their efforts toward this project.

[1] M. S. Shakeri *et al.*, *Sci. Rep.*, 12 (2022) 11950

[2] M. S. Shakeri *et al.*, *Adv. Funct. Mater.*, 43 (2023) 2304359

FLASH TALK, TUE./18:33

Liquid crystalline glassformer forming hexatic smectic X_A^* glass – DFT calculations for interpretation of X-ray diffraction and IR spectroscopy data

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The chiral mesogenic compound, abbreviated as 3F7HPH6, forms on cooling four smectic phases: paraelectric SmA^* , ferroelectric SmC^* , antiferroelectric SmC_A^* and tilted hexatic SmX_A^* (SmF_A^* or SmI_A^*). SmX_A^* forms the glass below $T_g = 230-233$ K. During heating of the supercooled sample, one or two crystal phases (for 2 K/min or 5-20 K/min, respectively) are observed upon cold crystallization. The fragility index of this glassformer, determined from the α -relaxation time, is equal to 94.5 [1]. The tilt angle of molecules, measured by the electro-optic method, reaches 44° in the SmC_A^* phase [2]. By comparing the tilt angle with the smectic layer spacing, determined by X-ray diffraction, one can obtain the molecular length $L = 34 \text{ \AA}$ and shape parameter $\delta\Theta = 25^\circ$. The latter is an angle between two vectors: one connecting the terminal C and F atoms, and another describing the direction of the aromatic molecular core. The high $\delta\Theta$ value indicates that 3F7HPH6 molecules have a strongly non-linear shape. DFT calculations performed in Gaussian 16 [3] allow us to find the molecular models with L , $\delta\Theta$ close to the experimental values. The models are subsequently used for the calculation of theoretical IR spectra and assignment of the vibrational modes to the experimental IR absorption bands.

Acknowledgements: We thank Assoc. Prof. Wojciech Zając (IFJ PAN) for help with DFT calculations, performed in Ares supercomputer from the Academic Computer Centre Cyfronet AGH (PLGrid Infrastructure).

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FLASH TALK, TUE./18:37

Self-assembly behavior of difluoroterphenyl derivatives differing with the linking bridge type

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The self-assembly behaviour and crystallization kinetics of two liquid crystal compounds, each featuring a 2',3'-difluorosubstituted terphenyl mesogenic core, have been detailed [1]. Calorimetric studies indicate that the type of linking bridge influences the polymorphism of smectic phases. The CH2O.3 compound [2], which has a $-\text{CH}_2\text{O}-$ linking bridge paired with a longer methylene spacer, exhibits a chiral smectic phase with antiferroelectric properties (SmC_A^* phase). In contrast, the COO.6 liquid crystal [3], with a $-\text{COO}-$ linking bridge and a shorter alkyl chain, forms a chiral smectic phase with ferroelectric properties (SmC^* phase). Both compounds undergo crystallization upon slow cooling, while fast cooling results in the vitrification of a conformationally disordered crystal phase. Dielectric measurements indicate complex relaxation dynamics in the identified thermodynamic states, and DFT calculations help estimate the nature of these relaxation processes.

The discovered findings could be highly significant for future research into liquid crystals and their potential applications. However, further investigation is needed to explore the relationships between mesophase organization and the phenomena of crystallization and vitrification, as well as their crystallization kinetics.

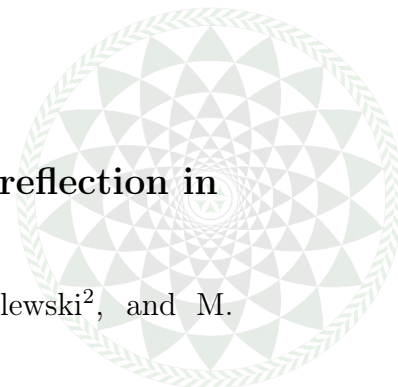
Acknowledgements: The PL-Grid Infrastructure and the ACC Cyfronet AGH (Krakow, Poland) are acknowledged for computational resources.

[1] A. Drzewicz *et al.*, Phys. Chem. Chem. Phys., 26 (2024) 8748

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FLASH TALK, TUE./18:41



Investigation of phase behaviour and selective light reflection in mixtures with azo compounds

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The multitude of existing and potential applications of liquid crystal materials highlights the crucial role of research on mesogenic multi-component systems. It makes it possible to design and predict the physicochemical properties of mixtures consisting of appropriately selected substances for which the phase sequence and phase transition temperatures are known. Detailed research using several experimental methods allows us to learn new ways of organizing molecules and observe the appearance or disappearance of certain mesophases and their stabilization in mixtures. Liquid-crystal thermography is one of the application examples, where selective light reflection can depend on the proportions of the mixture ingredients [1].

In this work, several two-component mixtures were prepared, containing various concentrations of individual components. The first component belongs to the mesogenic azo compound from the group of (E)-4-((4-alkyloxyphenyl)diazenyl)phenyl alkanoates (nOABOOCm, for n = 3,5,7,8,10 and m = 1-19), e.g., 3OABOOCm [2]. The second one is a chiral liquid-crystalline compound from the group of cholesteryl derivatives (e.g., cholesteryl pelargonate) or chiral azobenzene derivative (e.g., (E)-4-((4-undecylphenyl)diazenyl)phenyl 2-chloropropionate [3]).

Polarized Optical Microscopy (POM) and Differential Scanning Calorimetry (DSC) methods were used to determine the phase transition temperatures and thermal properties of such mixtures. On their basis, phase diagrams were prepared, for which an analysis of changes in the phase behaviour with changes in composition will be presented. The work also concerns selective light reflection investigation of mixtures using the POM method.

Acknowledgements: MP has been partly supported by the EU Project POWR.03.02.00-00-I004/16.

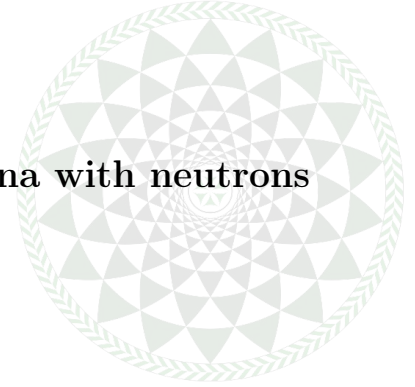
- [1] H.F. Gleeson, Thermography Using Liquid Crystals, in: edited by J. Goodby, et al., Handbook of Liquid Crystals Vol. 8, Academic Press Inc., New York (2014)
- [2] M. Piwowarczyk *et al.*, Thermochem. Acta, 731 (2024) 179649
- [3] A. Włodarczyk *et al.*, Proceedings SPIE, 3319 (1998) 40

MOLECULAR MAGNETS AND NANOMAGNETS

Chair: Javier Campo Ruiz

- 08:30 **Mark Johnson** (Grenoble, France)
New opportunities for studying multiscale phenomena with neutrons p. 38
- 09:05 **Mengmeng Wang** (Louvain-la-Neuve, Belgium)
Towards structural reorganization and stimulus responsiveness of single-molecule magnets and spin crossover complexes p. 39
- 09:35 **Marcin Sikora** (Kraków, Poland)
Insight into nucleation and growth processes with X-ray spectroscopy p. 40
- 10:05 **Illia Kozin** (Košice, Slovakia)
The field-induced Berezinskii–Kosterlitz–Thouless transition in a quasi 2D Heisenberg antiferromagnet $\text{Cu}[\text{C}_6\text{H}_2(\text{COO})_4][\text{C}_2\text{H}_5\text{NH}_3]_2$ on spatially anisotropic square lattice p. 41
- 10:20 **Bartosz Kłębowski** (Kraków, Poland)
The effect of cubic palladium nanoparticles (Pd NCs) surface modification on their cytotoxicity and radiosensitizing properties – in vitro studies p. 42

KEYNOTE, WED./08:30



New opportunities for studying multiscale phenomena with neutrons

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Neutron techniques cover many orders of magnitude in time and length scales, which can be extended even further by combining real time and space with reciprocal time and space techniques – neutrons are therefore perfectly suited to studying multiscale phenomena across a wide range of scientific fields. Since neutrons are scattered primarily by nuclei, the data gives unique insight into matter, materials and processes and is highly complementary to data from other experimental techniques. At the ILL, a major upgrade programme spanning eight years has just been completed. It has delivered about 30 projects for a budget of 60 M€ ensuring a state-of-the-art suite of instruments and scientific services for the decade to come. On average, the performance of each upgraded instrument has been increased by a factor of ten. The resulting, new opportunities for studying multiscale phenomena at ILL will be presented

INVITED TALK, WED./09:05

Towards structural eegulation and stimuli eesponsiveness of single-molecule magnets and spin crossover complexes

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To adapt to the current miniaturization of devices, single-molecule magnets (SMMs) and spin crossover (SCO) complexes carrying the potential of storage information at the molecular level have become the research hotspot. Systematical change of the structures and introducing external stimuli are beneficial to study the magneto-structural relationship and combine different physical properties. Metal-organic frameworks (MOFs) featuring structural diversity and porosity offer a promising platform for studying molecular nanomagnets. We reported for the first time of two Ln-MOFs showing switchable “on” and “off” SMM behaviors via temperature-induced reversible structural transformation [1]. A Dy^{III}–MOF featuring pore solvents responsive magnetization dynamics was studied, which was also applied to rapid and accurate sensing of p-xylene from the xylene isomers [2].

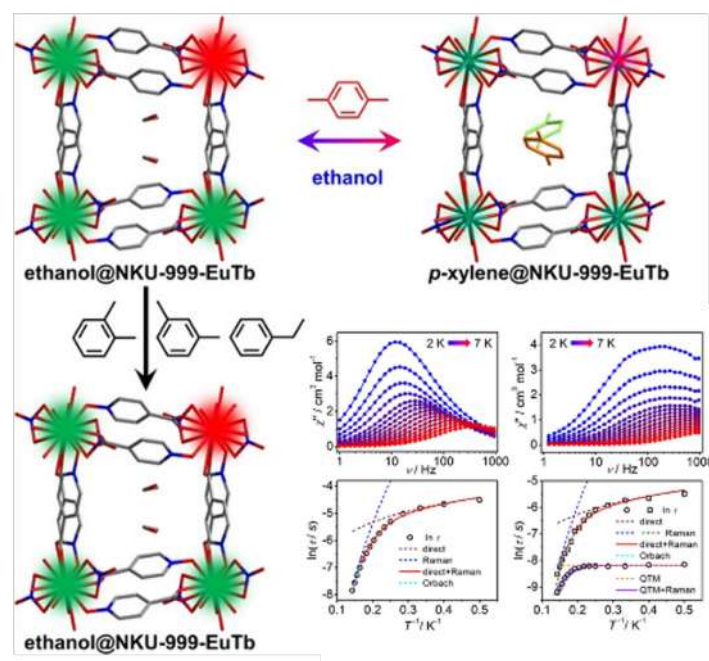


Figure 1: The luminescent and magnetic responsiveness of Ln-MOFs towards xylene isomers [2].

We are also doing some work aiming at achieving room temperature light induced spin state change [3] using the photoinduced 4+4 reversible cycloaddition of anthracene.

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INVITED TALK, WED./09:35



Insight into nucleation and growth processes with X-ray spectroscopy

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The construction of third generation synchrotron light sources has led to many advances in X-ray spectroscopy, including the growing number of in-situ experiments dedicated to probing of physico-chemical processes. After brief introduction to modern X-ray spectroscopy I will focus on its application to in-situ probing the processes of nucleation of metal and metal oxide clusters following the decomposition of metal-organic complexes. Results of two experiments will be discussed in details. The process of nucleation of metal clusters was investigated by ambient pressure X-ray photoelectron spectroscopy (AP XPS) during an ALD deposition of Cu films from Cu(hfac)₂ precursor. Experimentally determined evolution of coverage by and chemical state of Cu, F and C elements in the growing film was probed during adsorption and reduction steps of the ALD process to verify if clustering process is following the transmetalation reaction proposed by Dey and Elliot [1]. The process of nucleation and growth of magnetic iron oxide nanoparticles was probed in solution by means of core-to-core resonant X-ray emission spectroscopy (RXES). Spectra collected with circularly polarized light enabled an insight into the evolution of magnetic moment of the ensemble of growing nanoparticles by means of X-ray magnetometry [2]. We aimed to observe the transition from paramagnetic to superparamagnetic state at finite particle size as proposed by Bandow and Kimura [3] and to clarify the foundation of spin-ordering in nanoscale spinel iron oxides.

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CONTRIBUTED TALK, WED./10:05

The field-induced Berezinskii–Kosterlitz–Thouless transition in a quasi 2D Heisenberg antiferromagnet $\text{Cu}[\text{C}_6\text{H}_2(\text{COO})_4][\text{C}_2\text{H}_5\text{NH}_3]_2$ on spatially anisotropic square lattice

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Magnetic properties of the spin-1/2 quantum antiferromagnet $\text{Cu}[\text{C}_6\text{H}_2(\text{COO})_4][\text{C}_2\text{H}_5\text{NH}_3]_2$ were previously reported through susceptibility, magnetization and heat capacity measurements. Anisotropic exchange interaction with dominant intraplane coupling $J_1/k_B \approx 10$ K forms rectangular lattice with the anisotropy parameter $R = J_2/J_1 \approx 0.7$. No magnetic order state was observed down to 1.8 K [1].

We extended the heat capacity study in magnetic fields up to 9 T. A powder sample was measured in commercial Physical Property Measurement System (PPMS) device with ^3He insert at temperatures down to 0.4 K. In zero external field magnetic phase transition was still not evident down to the lowest temperature. Nevertheless, heat capacity peaks measured in magnetic field shifted towards lower temperatures. Consecutively, a magnetic phase diagram for $\text{Cu}[\text{C}_6\text{H}_2(\text{COO})_4][\text{C}_2\text{H}_5\text{NH}_3]_2$ was constructed, showing a fair agreement with quantum Monte Carlo simulation for the Berezinskii–Kosterlitz–Thouless (BKT) transition for spin-1/2 Heisenberg antiferromagnet on a square lattice. We also analyzed the magnetic entropy released near the BKT transition, associated with the unbinding of vortex-antivortex pairs. The released entropy slightly exceeded predictions for a square lattice, likely due to interlayer interactions.

Acknowledgements: The work was supported by the projects APVV-22-0172 and VEGA 1/0132/22.

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CONTRIBUTED TALK, WED./10:20

The effect of cubic palladium nanoparticles (Pd NCs) surface modification on their cytotoxicity and radiosensitizing properties – in vitro studies

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Finding new ways to fight cancer is an important medical challenge of today. The tumor cannot always be removed surgically, in turn classic radiotherapy and chemotherapy are associated with numerous side effects for the patient and the possibility of cancer cells becoming resistant to this type of treatment. As part of the research, the preparation of a cubic palladium nanocubes (Pd NCs) used as a radiosensitizers in simulated proton radiotherapy was proposed. Application of Pd NCs sensitizes the tumor to subsequent high-energy proton beam irradiation, further reducing the side effects of the therapy. Moreover, the application of Pd NCs instead of the more popular platinum or gold nanoparticles is economically viable, and the therapeutic effect is not less satisfactory.[1, 2] A successful attempt was also made to modify the Pd NCs with biocompatible polymers (PEG-Pd NCs), such as polyethylene glycol (PEG) in order to mask their cytotoxicity.[3] Furthermore, PEG-Pd NCs were covalently biofunctionalized with thio-glucose, obtaining nanomaterials with a larger ability to penetrate cancer cells (PEG-Glu-Pd NCs). The therapeutic effect of the obtained Pd NCs (both modified and non-modified) was tested on selected glioblastoma multiforme cell lines (LN229 and U118). These cells were cultured with a non-toxic concentration of Pd NCs and then irradiated by a proton beam. The survival of the cells subjected to this therapy was evaluated by the MTS test and flow cytometry analysis (annexin V assay). The obtained results showed a more satisfactory radiosensitizing effect when using functionalized nanosystems compared to unmodified Pd NCs.

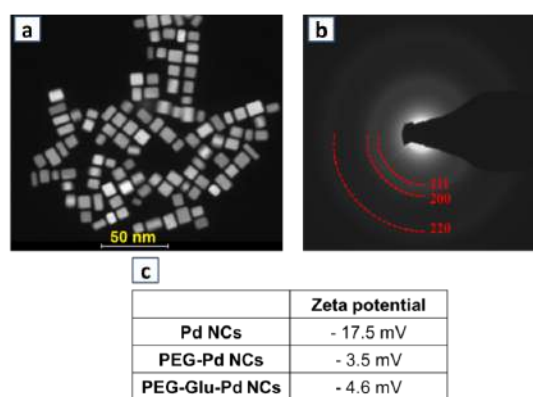


Figure 1: a) STEM overview image, b) SAED patterns of Pd NCs and c) zeta potential values of the (un)modified Pd NCs.

Acknowledgements: This research was funded by Polish National Science Centre, grant UMO-2020/37/N/ST5/02414. The authors thank the Institute of Engineering Materials and Biomaterials of the Silesian University of Technology, for the use of the Titan FEI TEM instrument.

[1] A. Abrishami *et al.*, *Commun. Biol.*, 7 (2024) 393

[2] Y-W. Jiang *et al.*, *Langmuir*, 36. (2020) 11637

[3] B. A. Zhaisanbayeva *et al.*, *Int. J. Pharmaceutics*, 652 (2024) 123852

COMPUTATIONAL PHYSICS

Chair: Neven Žitomir Barišič

	Pascal Simon (Orsay, France)	
11:05	Hund's assisted multi-channel quantum phase transition in the Fe(Se,Te) superconductor	p. 44
	Dominik Legut (Ostrava, Czech Republic)	
11:40	Magnetostriction of polycrystalline terfenol-D – effect of grain morphology and orientation	p. 45
	Natalia Osiecka-Drewniak (Kraków, Poland)	
12:10	Using neural networks to study liquid crystal textures	p. 46
	Athanasios Koliogirgos (Prague, Czech Republic)	
12:25	An ab-initio theory of inelastic electron tunneling spectrum of vibrating magnetic molecules adsorbed on superconductors	p. 47
	Ha Nguyen (Kraków, Poland)	
12:40	DFT study of optical properties and pressure dependence of electronic density of state in double perovskite Ba ₂ TiMnO ₆	p. 48

KEYNOTE, WED./11:05

Hund's assisted multi-channel quantum phase transition in the Fe(Se,Te) superconductor

P. Simon

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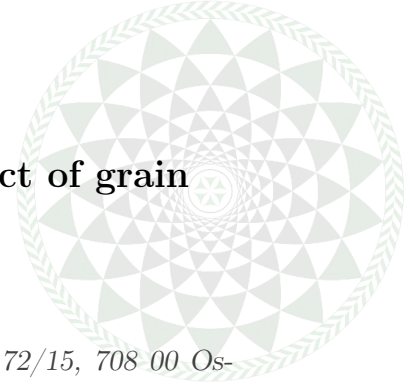
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Understanding the interplay between individual magnetic impurities and superconductivity is crucial for bottom-up construction of novel phases of matter, as well as to exploit the local response as a probing tool. For decades, the description by Yu, Shiba and Rusinov (YSR) of single spins in a superconductor and its extension to include quantum effects has proven highly successful: the pair-breaking potential of the spin generates sub-gap bound states. I will first show how atomically-resolved shot noise can be used to reveal the coherent and incoherent dynamics of such sub-gap bound states [1]. By tuning the energy of the sub-gap states through zero, the impurity screening by the superconductor makes the ground state gain or lose an electron, signalling a parity breaking quantum phase transition. I will present a set of scanning tunneling microscopy (STM) measurements that explicitly invalidate the classical YSR paradigm, and propose an interpretation in terms of a multi-orbital Anderson impurity model [2]. In particular, I show that in multi-orbital impurities, electronic correlations can conversely lead to a quantum phase transition where the impurity mean occupation changes dramatically, without significant effect of the screening by the superconductor. This finding implies that the YSR treatment is not always valid, and that intra-atomic interactions, particularly Hund's coupling that favours high-spin configurations, are an essential ingredient for understanding the sub-gap states.

[1] U. Thupakula *et al.*, Phys. Rev. Lett. 128, (2022), 247001

[2] M. Uldemolins *et al.*, (2023), arXiv:2310.06030.

INVITED TALK, WED./12:10



Magnetostriction of polycrystalline terfenol-D – effect of grain morphology and orientation

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Magnetoelastic interactions are responsible for many interesting phenomena such as Joulemagnetostriction, the Wiedemann effect, the Villari effect, effects on sound velocity, and many others. In this work [1], we investigate the effect of microstructure on saturation magnetostriction of Terfenol-D ($\text{Tb}_{0.27}\text{Dy}_{0.73}\text{Fe}_2$) by means of Finite Element Method. The model is based on the equilibrium magnetoelastic strain tensor at magnetic saturation, and shows that the crystal orientation jointly with the grain volume fraction play a more significant role on saturation magnetostriction than the morphology of the grains. We also calculate the dependence of saturation magnetostriction on the dispersion angle of the distribution of grains in the oriented growth crystal directions $\langle 011 \rangle$ and $\langle 111 \rangle$. This result evinces the importance of high-quality control of grain orientation in the synthesis of grain-aligned polycrystalline Terfenol-D. The input parameters, i.e. magnetostriction coefficients (λ_{100} and λ_{111}), could be determined using novel developed method [2] based on the first-principles calculations (microscopic scale) combined with classical spin-lattice simulations [3] (mesoscopic scale) within a multiscale approach.

[1] P. Nieves, and D. Legut, Solid State Comm., 352 (2022) 114825.

[2] P. Nieves, D. Legut et al, Comput. Phys. Comm., 271 (2022) 108197.

[3] P. Nieves, D. Legut et al, Phys. Rev. B, 103 (2021) 094437.

CONTRIBUTED TALK, WED./12:10

Using neural networks to study liquid crystal textures

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The optical birefringence of molecules exhibiting liquid crystal phases allows for the observation of textures in polarized light. The observed texture pattern depends on various factors, including the thickness of the liquid crystal layer, the type of glass material used, the nature of the coating material, the quality of the glass plates, the temperature gradient in the system, mechanical stresses in the sample, as well as the influence of external magnetic or electric fields [1]. Therefore, depending on these factors, a given liquid crystal phase can exhibit different textures. It is possible to identify liquid crystal phases by observing their textures, although this requires significant experience from the observer. Texture investigations provide information on both phase transition temperatures and the type of phase.

In the proposed presentation, we will demonstrate how machine learning algorithms handle the differentiation of liquid crystal textures of 3F7HPhH7 substance. Results utilizing the Local Binary Pattern (LBP) algorithm and convolutional neural networks will be presented [2, 3]. The developed models achieved a high 95% differentiation rate for the following phases: SmA, SmC*, SmCA*, and the glassy state of the SmCA* phase. This approach makes the differentiation of liquid crystal textures objective and independent of the researcher's visual sensitivity.

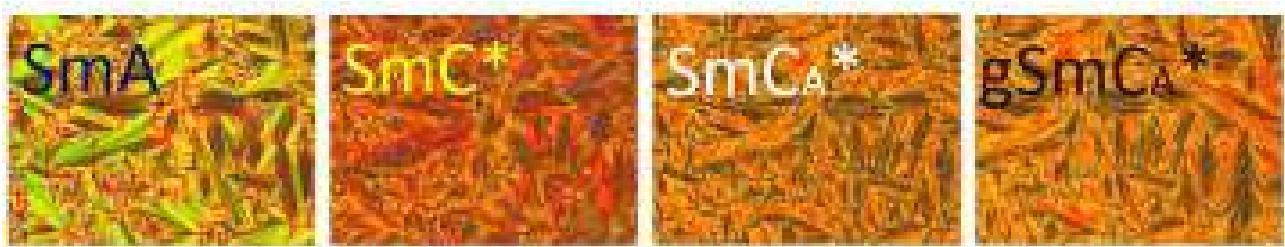


Figure 1: Example of textures of smectic A phase (SmA), ferroelectric smectic C phase (SmC*), antiferroelectric smectic C (SmCA*) and glass of antiferroelectric smectic C phase (gSmCA*).

[1] N. Osiecka-Drewniak *et al.*, *Liq. Cryst.*, 51 (2024) 128

[2] N. Osiecka-Drewniak *et al.*, *Liq. Cryst.*, 51 (2023) 255

[3] N. Osiecka-Drewniak *et al.*, *Soft Matt.*, 20 (2024) 2400

CONTRIBUTED TALK, WED./12:25

An ab-initio theory of inelastic electron tunneling spectrum of vibrating magnetic molecules adsorbed on superconductors

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We present an efficient method of calculating the vibrational spectrum of a magnetic molecule adsorbed on a superconductor, directly related to the first derivative of the tunneling IV curve. The work is motivated by a recent scanning-tunneling spectroscopy of lead phthalocyanine on superconducting Pb(100), showing a wealth of vibrational excitations, the number of which highly exceeds molecular vibrations typically encountered on normal metals.[1] We design a minimal model which represents the inelastic transitions by the spectral function of a frontier orbital of the molecule in isolation. The model allows for an exact solution; otherwise the full correlated superconducting problem would be hard to treat. The model parameters are supplied from an ab-initio calculation, where the presence of the surface on the deformation of molecular geometry can be taken into account. The spectral function of the highest-occupied molecular orbital of the anionic $PbPc^{1-}$ shows the best agreement with the experimental reference among other molecular charge states and orbitals. The method allows to include multiple vibrational transitions straightforwardly.

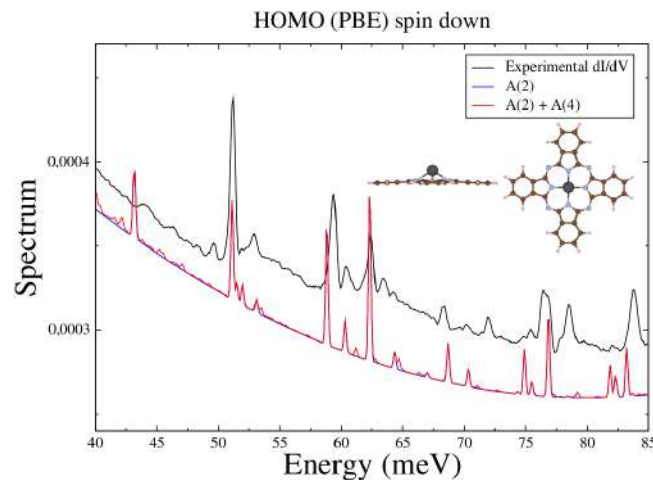
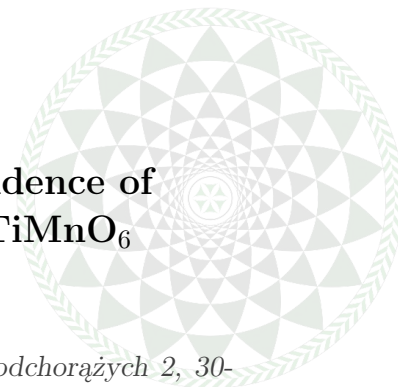


Figure 1: Spectral function describing single and double electron-vibrational transitions from the minority-spin molecular orbital HOMO of $PbPc^{1-}$ using the PBE functional. The experimental dI/dV spectrum from Ref.[1] is included. To facilitate comparison, a polynomial background has been added to the theoretical spectrum. Inset shows the C_{4v} geometry of PbPc relaxed on top of Pb(100), employed in the calculation.

[1] J. Homberg *et al.*, Phys. Rev. Lett., 129 (2022) 116801

CONTRIBUTED TALK, WED./12:40



DFT study of optical properties and pressure dependence of electronic density of state in double perovskite $\text{Ba}_2\text{TiMnO}_6$

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Double perovskite compounds have gotten a lot of attention in recent years due to their useful features and possible uses in magnetocaloric and optoelectronic devices [1, 2]. In this study, we present optical properties and pressure dependence of electronic density of state obtained from the Density Functional Theory (DFT) calculations for semiconducting double perovskite $\text{Ba}_2\text{TiMnO}_6$, using PBE-GGA and GGA+U exchange-correlation functionals. Following our prior research, we discovered that $\text{Ba}_2\text{TiMnO}_6$ is a direct semiconducting band gap of 0.98 eV (PBE-GGA) and 1.23 eV (GGA+U) [3]. The optical calculations show high dielectric constants, a strong light absorption coefficient in the UV range, and a significant optical conductivity of $6.53 \times 10^5 \text{ cm}^{-1}$, suggesting potential for high-performance perovskite solar cells in optoelectronic applications. The study discovered that optical features below 15 eV in PBE-GGA and GGA+U calculations are primarily attributable to intraband and interband transitions of Mn-3d electrons. Using the Projected Augmented Wave (PAW) approach, we also investigated the impact of pressure on crystal structure and density of state. Our findings show that under compressive strain at pressures around 8 GPa, structural distortion may occur, as well as a significant increase in the semiconducting gap.

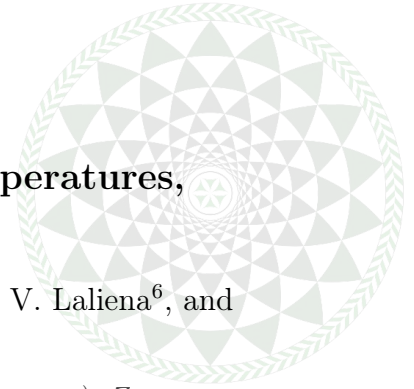
- [1] E. Greul *et al.*, J. Mater. Chem. A, 5 (2017) 19972
- [2] W. Yin *et al.*, Energy Environ. Sci., 12 (2019) 442
- [3] T. T. H. Nguyen *et al.*, J. Magn. Magn. Mater., 587 (2023) 171274

MOLECULAR MAGNETS AND NANOMAGNETS

Chair: Beata Nowicka

- Javier Campo Ruiz** (Zaragoza, Spain)
08:30 SANS and μ SR studies on the new state at low temperatures, "B-Phase", in MnSi p. 50
- Jan van Leusen** (Aachen, Germany)
09:05 About the magnetism of coordination compounds – from 3d to 5f metals p. 51
- Ján Titiš** (Trnava, Slovakia)
09:35 Advances in single-molecule magnets: investigating slow magnetic relaxation and its mechanisms p. 52
- Wiktor Wolański** (Kraków, Poland)
10:05 The new family of photomagnetic coordination frameworks based on $[\text{Mo}(\text{CN})_7]^{4-}$ building blocks p. 53
- Oliwia Polit** (Kraków, Poland)
10:20 Magnetic Ni@Au and Co@Au nanocomposite particles synthesised by laser ablation in liquid p. 54

KEYNOTE, THU./08:30



SANS and μ SR studies on the new state at low temperatures, "B-Phase", in MnSi

M. Pardo-Sainz^{1,2}, M. Mito³, K. Ohishi⁴, Y. Kousaka², K. Kojima⁵, V. Laliena⁶, and J. Campo¹

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Recently, we suggested theoretically, that at low T the conical (CH) and forced-ferromagnetic (FFM) phases in cubic helimagnets, are not connected but are separated by another Skyrmion Lattice phase (SkL), which could be metastable, and a new phase of unknown nature just below the critical field H_c at low T [1]. The theoretical prediction of the new SkL phase at low T is in good agreement with the experiments reported in ref [2]. On the other hand, by using careful ac susceptibility at low temperature, we determined the magnetic phase diagrams of oriented crystals of MnSi [3] in which a new phase (B-phase) emerges which could be consistent with the theoretical prediction for the new unknown low temperature phase.

In order to clarify the nature of this B-phase at low T near critical field, we performed SANS and muon spin rotation (μ SR) measurements. At high magnetic field, in configuration $H // [111] \perp ki$, the SANS patterns show two peaks along the horizontal axis which are identified as the magnetic Bragg peaks of the conical state. On the other hand, no diffraction peaks were observed for $H // [111] // ki$, in which, for example, a six-fold-symmetric diffraction pattern due to a formation of SkL is observed in the SkL region. These results suggest the CH phase exists in B-phase being different from the A-phase near T_c . According to the μ SR results, we found the internal magnetic field distribution in B-phase is apparently different from that in CH at low fields and FFM phases, consistent with the SANS results, and indicating an internal rotation of helices at high magnetic fields and low temperatures.

In the presentation, we will talk about the results of both SANS and μ SR in detail, and discuss a spin texture in B-phase.

[1] V. Laliena & J. Campo, Phys. Rev. B 96, (2017) 134420.

[2] T. Nakajima *et al.*, Phys. Rev. B 98, (2018) 014424.

[3] M. Ohkuma *et al.*, APL Mater. 10, (2022) 041104.

INVITED TALK, THU./09:05

About the magnetism of coordination compounds – from 3d to 5f metals

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Unravelling the magnetism of molecular compounds can be rather straightforward or exceptionally challenging depending on the type of ligands, the coordination geometry of the magnetic center and, in particular, the electronic properties of the central metal. In general, contributions to be considered arise from spin-orbit coupling, interelectronic repulsion and the ligand-field potential. While for most 3d elements one or two of these contributions can be either neglected or treated in an effective model, the heavier the central metal element (4f or 5f), the less simplifications are viable. To shed some light on the electronic behavior of coordination compounds and the resulting magnetism, the computational framework CONDON [1] is employed to calculate and visualize the corresponding physical results and repercussions.

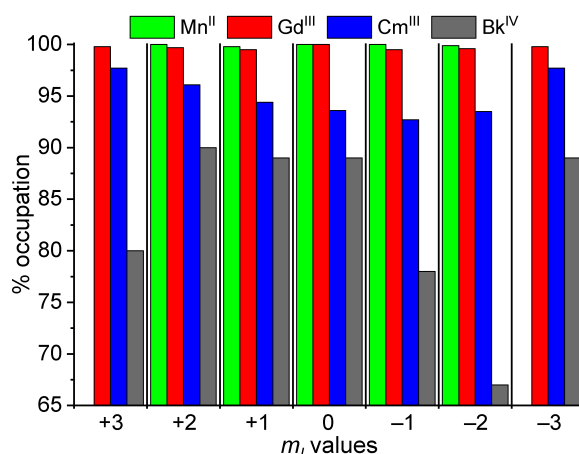


Figure 1: Electron occupation of (complex) d or f orbitals of ${}^6S_{5/2}$ or ${}^8S_{7/2}$ terms, respectively.



[1] M. Speldrich *et al.*, J. Comput. Chem., 39 (2018) 2133

INVITED TALK, THU./09:35

Advances in single-molecule magnets: investigating slow magnetic relaxation and its mechanisms

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The drive to miniaturize electronic devices and the quest for higher information storage capacity have pushed modern hard-drive technology to the brink of the superparamagnetic limit. Surpassing this limit requires either the development of new classes of information storage materials or fundamental improvements in current technology. Single-molecule magnets (SMMs), with their well-defined nanosized inorganic cores encapsulated by organic shells, represent a significant advancement in the miniaturization of future memory devices [1]. Detection of slow magnetic relaxation (SMR) in metal complexes is an important task in the emerging field of molecular magnetism. SMMs, as the main objects of interest, show SMR as a consequence of the energy barrier E_b for the magnetization reversal between the two lowest $M_S = \pm S$ states. We have investigated a number of metal complexes by the AC susceptibility measurements in order to identify an SMR based on the temperature and frequency dependence of the out-of-phase magnetic susceptibility (Fig. 1). The studied systems cover 3d and 4f systems with different topology of magnetic centers. In certain cases, the reciprocating thermal behavior is detected. On cooling, the slow relaxation time is prolonged until a certain limit and then, unexpectedly, is accelerated. The low-temperature magnetic data can be successfully fitted by assuming Raman and/or phonon bottleneck mechanisms of the slow magnetic relaxation for the high-frequency relaxation channel. An additional term with the negative temperature exponent can reproduce the whole experimental data set.

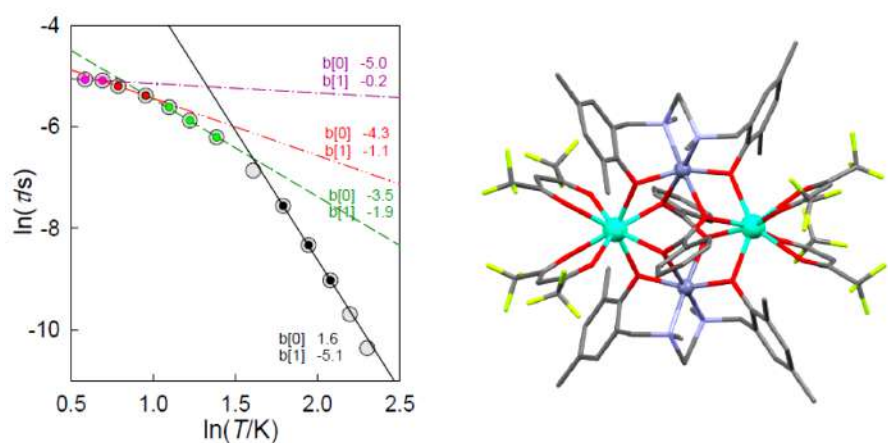


Figure 1: Different contributions to the relaxation time in $[\text{Dy}_2^{\text{III}}\text{Zn}_2^{\text{II}}]$ complex [2]

Acknowledgements: Slovak grant agencies (APVV 19-0087 and VEGA 1/0086/21) are acknowledged for the financial support.

[1] V. Vieru *et al.*, *Angew. Chem. Int. Ed.* 63 (2024) e202303146.

[2] S.M.T. Abtab *et al.*, *Inorg. Chem.* 53 (2014) 1295–1306.

CONTRIBUTED TALK, THU./10:05

The new family of photomagnetic coordination frameworks based on $[\text{Mo}(\text{CN})_7]^{4-}$ building blocks

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Polycyanometallates are well-known as building blocks for the construction of coordination frameworks which show magnetic or photomagnetic behavior and other effects such as SGH, luminescence, SCO, porosity, etc.[1] We recently discovered that potassium heptacyanomolybdate(III) can be an excellent precursor for designing photomagnetic systems due to its intrinsic spin state photoswitching behavior, high relaxation temperature of the photoexcited state and reverse photoswitchability after irradiation with a different wavelength.[3] During our ongoing research, four coordination systems based on manganese(II), imidazole and heptacyanomolybdate(III) were discovered and characterized structurally and magnetically. Their spectroscopic properties and photomagnetic behavior was also investigated.[2] All four compounds show long range magnetic ordering and it was discovered that upon 405 nm irradiation the magnetic ordering temperature (T_c) increases in each case. The underlying photoswitching mechanism is associated with the photodissociation of one of the cyanide ligands from the low-spin $[\text{Mo}(\text{CN})_7]^{4-}$ followed by the formation of a high spin $[\text{Mo}^{\text{III}}(\text{CN})_6]^{3-}$.

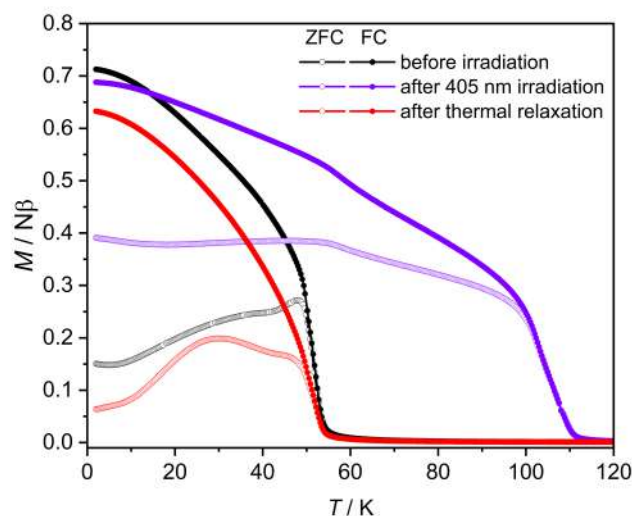


Figure 1: ZFC-FC curves at 50 Oe for the compound $[\text{Mn}^{\text{II}}(\text{imidazole})_2][\text{Mo}^{\text{III}}(\text{CN})_7]_n$ before and after irradiation with 405 nm light and after thermal relaxation at 350 K.

Acknowledgements: This research was funded by the European Research Council (ERC) under the EU Horizon Europe research and innovation programme, project LUX-INVENTA, grant agreement no 101045004.

- [1] S. Chorazy *et al.*, Chem. Rev., 124 (2024) 5930
- [2] M. Magott *et al.*, Dalton Trans., 48 (2019) 15493
- [3] Manuscript in preparation

CONTRIBUTED TALK, THU./10:20

Magnetic Ni@Au and Co@Au nanocomposite particles synthesised by laser ablation in liquid

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Composites nanoparticles can merge features of few materials, as well as lead to exhibit new properties, which makes that kind of materials very attractive for applications in many fields of science, technology and industry. One of the alternatives to commonly used procedures of nanoparticle's preparation is Pulsed Laser Ablation in Liquid (PLAL). Laser ablation in liquid can be used to generate nanoparticles from many solid materials and change of laser parameters and process conditions allows creating particles with different size, chemical composition, morphology or structure. Typically, in PLAL set-up a bulk target material is immersed in a solvent and irradiated with high energy, focused laser beam. For this project we implemented a modified method to ablate targets in the presence of nanoparticles in solvent. This way we created a few nickel-gold and cobalt-gold composites systems. Magnetic hysteresis loops of two Ni and Au based samples are shown in Fig. 1. We show how modification of laser synthesis conditions can change physical properties, including magnetic properties of the systems.

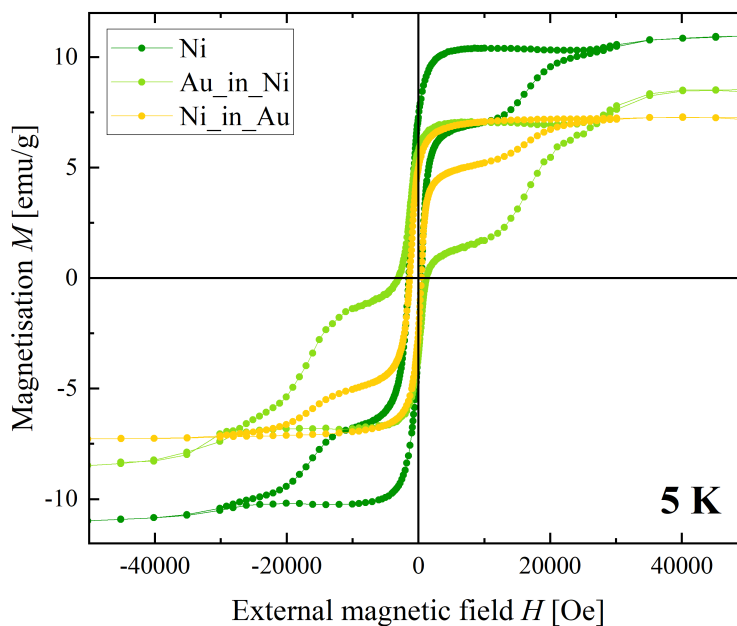


Figure 1: Magnetic hysteresis loops of two Ni and Au based composite nanoparticles and Ni nanoparticles shown as a reference, measured in low temperature

Acknowledgements: This research was supported by a French Government Scholarship.

MISCELLANY

Chair: Przemysław Piekarz

- 11:00 **Ubirajara van Kolck** (Trento, Italy) p. 56
The discrete charm of scale invariance
- 12:00 **Oleksandr Tomchuk** (Didcot, UK) p. 57
Structural organization of confined liquid crystals revealed by scattering techniques
- 12:30 **Adam Sieradzki** (Wrocław, Poland) p. 58
Hybrid Perovskites: exploring the thin line between order and disorder
- 13:00 **Grzegorz Dziembaj** (Kraków, Poland) p. 59
Few-body electron-hole photoluminescence spectra under the off-resonant THz-frequency laser beam irradiation
- 13:15 **Svitlana Pastukh** (Kraków, Poland) p. 60
First-principles analysis of anharmonic effects on thermal transport in graphene and h-BN

SPECIAL LECTURE, THU./11:00

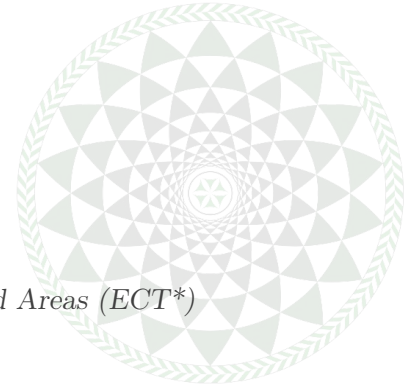
The discrete charm of scale invariance

U. van Kolck

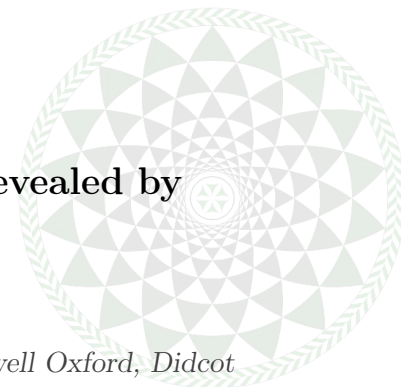
European Centre for Theoretical Studies in Nuclear Physics and Related Areas (ECT)*

email:

Nature is certainly not invariant under changes of scale. Phenomena and laws are characterized by parameters that determine their physical dimensions. However, while the complexity of some many-body systems may stem from a profusion of distinct scales, rich structures (such as fractals) exist even when there is no more than one essential scale associated with *discrete* scale invariance. I will discuss how intrinsically quantum-mechanical structures with unique properties, sometimes labeled "Efimov physics", emerge in nuclear and some closely related atomic systems from a contact three-body force.



INVITED TALK, THU./12:00



Structural organization of confined liquid crystals revealed by scattering techniques

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²The Henryk Niewodniczański Institute of Nuclear Physics, Polish Academy of Sciences, Kraków 31-342, Poland

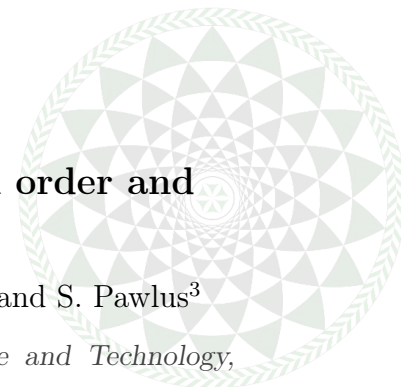
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Due to the specific physical phenomena and potential applications, confined liquid crystals (LCs) have been actively studied using dielectric, calorimetric, and optical methods. It has been indicated that geometrical restrictions ranging from nanopores to micropores significantly affect the morphology and dynamics, leading to reduced phase transition temperatures and sometimes to their complete suppression, depending on the pore size and host matrix elasticity [1, 2]. "Hard" spatial confinement is provided by various porous materials, such as anodic aluminum oxide (AAO) with cylindrical channels providing 2D confinement [3]. Another way to achieve nanoconfinement is the synthesis of nanofilms of LC materials, for example, using molecular beam deposition. In this case, one obtains 1D confinement. Our research project primarily focused on *n*CFPB and *n*BT compounds. In this study, we applied neutron and X-ray small-angle scattering (SANS & SAXS) as well as specular reflectometry (NR & XRR) to analyze the molecular ordering in cylindrical pores and thin film geometries for various LCs over a wide range of diameters and thicknesses, respectively. The results support the paranematic ordering of LC molecules close to the boundaries of nanosized pores, while no effect was observed for 200 nm pores. In the case of nanofilms, smectic ordering was observed over the entire studied range from tens to hundreds of nanometers.

Acknowledgements: Ultra-SANS experiments were carried out at the CANAM infrastructure of the NPI CAS Řež. The employment of the CICRR infrastructure supported by MEYS project M2023041 is acknowledged. SANS measurements based on the infrastructure of Budapest Neutron Centre are also gratefully acknowledged. The author is grateful to the Science and Technology Facilities Council for access to the OFFSPEC neutron reflectometer as well as the SAXS and XRR instruments at the Materials Characterisation Laboratory at ISIS.

- [1] M. Jasiurkowska-Delaporte *et al.*, *J. Mol. Liq.*, 308, (2020), 113039
- [2] M. Jasiurkowska-Delaporte *et al.*, *J. Mol. Liq.*, 331, (2021), 115817
- [3] E. Juszyńska-Gałązka & W. Zając, *Phase Transit.*, 96, (2023), 89-96

INVITED TALK, THU./12:30



Hybrid Perovskites: exploring the thin line between order and disorder

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Hybrid organic-inorganic perovskites have risen as a dynamic class of compounds, boasting customizable optoelectronic traits and an array of potential applications. This material family exhibits a diverse array of lattice dynamics and intricate dielectric responses. The alignment of polar molecular cations induced by external fields, defying their usual thermal fluctuations, instigates orientational polarization, underlying active relaxation phenomena.

Although dielectric relaxation processes are predominantly associated with disordered high-temperature phases of hybrid organic-inorganic compounds, they often dissipate upon transitioning to structurally-ordered low-temperature (LT) states. Remarkably, only a handful of hybrid compounds retain dielectrically-active residual relaxation dynamics of molecular cations in the LT phase, the origin of which remains elusive.

This study aims to probe deeper into the realm of low-temperature disorder and dynamics within hybrid perovskite-like systems, examining a range of compound examples. Employing X-ray diffraction (XRD), Raman spectroscopy, and broadband dielectric spectroscopy (BDS), we unveil that the first-order structural transformation from order to disorder does not entirely quash molecular dynamics within the organic building blocks. We will scrutinize this motion's mechanism and its implications for the optoelectronic properties of these materials.

CONTRIBUTED TALK, THU./13:00

Few-body electron-hole photoluminescence spectra under the off-resonant THz-frequency laser beam irradiation

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The electron-hole (eh) few-body complexes like excitons and trions are bound quasiparticles with characteristic binding energies dependent on the individual orbital energies of constituent particles as well as the attractive (eh) and repulsive (ee) interaction energies. Analysis made in Hennerberger-Kramers frame of reference [1, 2] shows that under irradiation with off-resonant THz-frequency laser the former is renormalized due to anti-phase oscillations of eh pair while the latter is left unchanged. Such selective light-matter coupling to some parts of eh system paves the way towards effective manipulation of its photoluminescence spectra in reversible and repetitive way fulfilling hence the assumptions of the Floquet engineering [3]. Here we consider the exciton and the trion confined in 100-nm-long InGaAs quantum wire coupled to off-resonant 500-THz laser beam. Although the reduced dimensionality of confinement enhances the correlations effects, the coupling to photon field may overwhelms the eh correlation energy what finally results in gradually increased energies of quasiparticles states accompanied with continuously lowered oscillator strength of the bright states both being the hallmarks of the optically induced Stark effect.

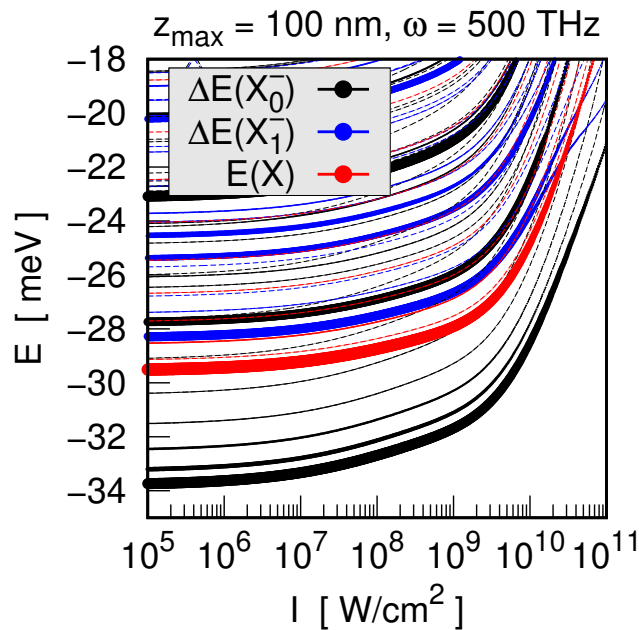


Figure 1: Optical spectrum of neutral and negatively charged trion confined in a 100-nm-long quantum wire irradiated with off-resonant 500-THz laser beam. Width of each line corresponds to oscillator strength of energy level.

- [1] T. Chwiej *et al.*, J. Phys. Condens. Matter., 35 (2023) 355302
- [2] I. V. Iorsh *et al.*, Phys. Rev. B, 105 (2022) 165414
- [3] T. Oka *et al.*, Annu. Rev. Condens. Matter Phys., 10 (2019) 387

CONTRIBUTED TALK, THU./13:15



First-principles analysis of anharmonic effects on thermal transport in graphene and h-BN

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Graphene and hexagonal boron nitride (h-BN) have emerged as quintessential examples of two-dimensional van der Waals layered materials, exhibiting significant anisotropy in their physical properties. In our study we present a comparative analysis of the lattice dynamical properties and thermal conductivity of graphene and h-BN bilayers, incorporating anharmonic corrections. Utilizing first-principles computational methods based on density functional theory (DFT) and atomic force determinations, we capture atomic vibrations in the harmonic approximation and assess anharmonicity using the temperature-dependent effective potential approach. Structure optimization was performed using VASP[1], while anharmonic calculations were conducted with HECSS[2] and ALAMODE[3] tools. Our results highlight the significant influence of anharmonicity in h-BN calculations, elucidating the impact of factors such as LO-TO splitting and higher-order anharmonic corrections on thermal transport. Additionally, our data show good agreement with experimental measurements, providing critical insights into the thermal conductivity behavior in bilayer structures and laying the groundwork for future research.

[1] G. Kresse *et al.*, Phys. Rev. B, 54 (1996) 11169

[2] T. Tadano *et al.*, J. Phys. Condens. Matter, 26 (2014) 225402

[3] P. T. Jochym *et al.*, SciPost Phys., 10 (2021) 129

SOFT MATTER AND GLASS FORMERS

Chair: Ján Titiš

14:50	Beata Nowicka (Kraków, Poland) Composites of a multistable and multiswitchable coordination chain	p. 62
15:25	Sebastian Pawlus (Chorzów, Poland) Supramolecular structures in monohydroxy alcohols: new group of halogen alcohols	p. 63
15:55	Yasuhiro Nakazawa (Toyonaka/Osaka, Japan) Hole-doped quantum spin liquid in Dimer-Mott organic compounds	p. 64
16:25	Daniele Sonaglioni (Pisa, Italy) PLX4720: new perspectives in an anticancer drug	p. 65

KEYNOTE, THU./14:50

Composites of a multistable and multiswitchable coordination chain

B. Nowicka¹, M. Fitta², A. Pacanowska², and G. Wota¹¹Jagiellonian University, Faculty of Chemistry, Gronostajowa 2, 30-387 Kraków, Poland²Institute of Nuclear Physics Polish Academy of Sciences, Radzikowskiego 152, 31-342 Kraków, Poland

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Switchability based on the change in electronic states of metal ions, which results in the change of color and magnetic susceptibility, is an interesting feature observed in some coordination networks. To utilize its application potential, it is essential to overcome the drawbacks arising from the crystalline form of the compounds, which are usually brittle and often show poor surface stability. Embedding in organic polymer matrix to form composites is a promising pathway to achieve surface protection and favorable mechanical properties.

The $\text{NH}_4[\text{Ni}(\text{cyclam})][\text{Fe}(\text{CN})_6] \cdot 5\text{H}_2\text{O}_n$ chain (**1**) is a remarkable coordination polymer, which shows multistability and multiswitchability related to the metal-to-metal charge transfer process (MMCT) [1]. At ambient conditions it can coexist in three different phases (Fig. 1): red HT, blue LT, and greenish-yellow dehydrated phase (Deh). The switching between them can be controlled by temperature, pressure, and humidity changes. Although **1** can be subjected to repeated phase transitions, which include exposure to high humidity, it is extremely fragile to contact with liquid water, upon which it recrystallizes to an MMCT-inactive 2D network. To protect it from water damage we dispersed **1** in an organic polymer matrix using hydrophobic polycaprolactone (PCL). The resulting composite material in the form of foil or electrospun mat can be immersed in water for 24 hours without deterioration. At the same time, it is water vapor permeable and retains the switchability by humidity changes. Preventing dehydration by air-tight sealing allows the application of the composite foil for heat-removable writing, effected by pressure-induced switching from HT to LT phase (Fig.1).

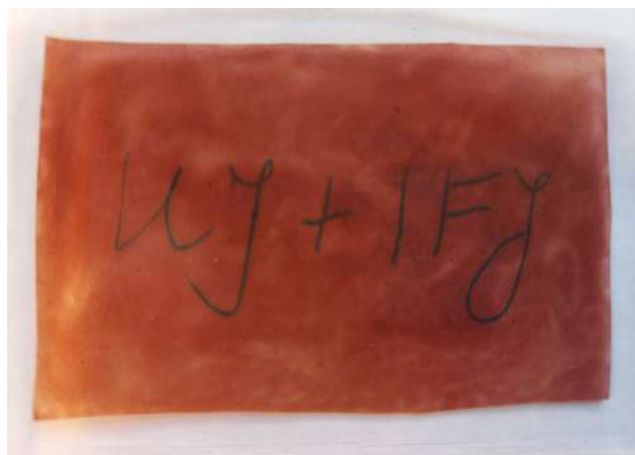
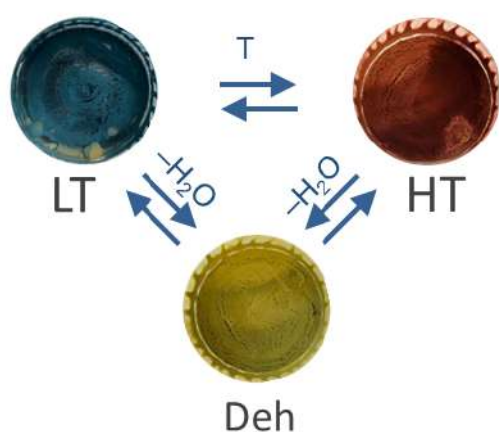


Figure 1: Three phases of **1** (left), pressure writing on the composite **1**/PCL foil (right).

[1] M. Reczyński *et al.*, *Angew. Chemie - Int. Ed.*, 60, (2021), 2330-2338

INVITED TALK, THU./15:25

Supramolecular structures in monohydroxy alcohols: new group of halogen alcohols

S. Pawlus¹, K. Łucak¹, A. Z. Szeremeta¹, J. Grelska¹, K. Jurkiewicz¹, N. Soszka¹, B. Hachuła², S. Kołodziej³, R. Wrzałik¹, and K. Kamiński¹

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Monohydroxy alcohols (MA), due to their unique physical and chemical properties and close similarity to water, are at the center of attention to many research groups. One of their most fascinating features is an exponential response function—called Debye (D) relaxation, a slower-than-structural-one - a source of hot scientific debate. It is commonly observed in dielectric measurements of aliphatic MAs. According to current knowledge, the dynamic properties of the D process for associating liquids reflect their complex internal structure, which is driven by the formation of chain-like supramolecular clusters through hydrogen bonds (HBs). To find a deeper connection between the dynamical properties of the D process and the architecture or size of the supramolecular associates, most authors focused their attention on the investigations of the two basic classes of monohydroxy alcohols. The first one obeys alcohols differing in the position of the OH group in the carbon skeleton or the chain length of the backbone with a constant location of the OH group. The second category of alcohols includes molecules in which the attached large functional group, like a phenyl group, is devoid of the dipole moment and behaves as a steric hindrance, preventing the formation of effective HBs. Surprisingly, much less is done on systems like halogen alcohols, where an additional dipole moment comparable to the one generated by the hydroxyl moiety already exists in the structure.

During the presentation, I will demonstrate similarities and differences between “ordinary alcohol”, n-propanol, and its halogen derivatives: 3-chloro-1-propanol, 3-bromo-1-propanol, and 3-iodo-1-propanol (Fig. 1) and their isomers studied with different experimental methods, at both ambient [1] and high-pressure conditions.

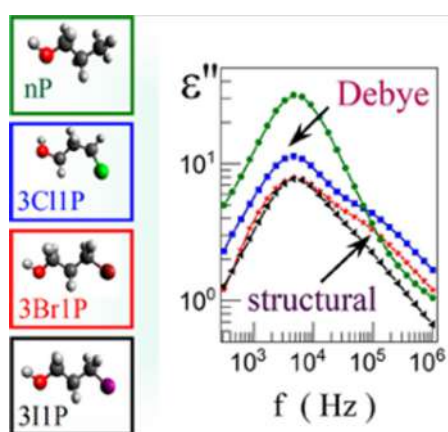


Figure 1: Comparison of the dielectric loss spectra of n-propanol and its halogen derivatives

Acknowledgements: The presentation is financially supported by the National Science Centre, Poland, OPUS 18 (No.: UMO-2019/35/B/ST3/02670).

[1] K Łucak et. al., J. Phys. Chem. B, 127 (2023) 9102.

INVITED TALK, THU./15:55



Hole-doped quantum spin liquid in Dimer-Mott organic compounds

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The molecular-dimer Mott insulating states revealed in organic charge transfer complexes with quasi-two-dimensional (quasi-2D) structures tend to form antiferromagnetic ordering at low temperatures. However, those in frustrated structures for example in 2D triangle lattices or Kagome lattices prevent the long-range ordering and so-called quantum spin liquid emerges. The doping of hole or electron carriers can change the Mott insulating state to an exotic metallic state which sometimes produces unconventional superconducting ground state.

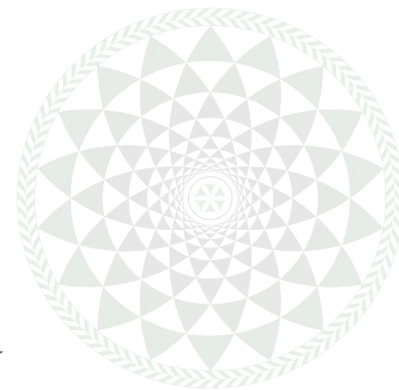
In this talk, we report novel features of a frustrated molecule-based charge transfer complexes with carrier doping investigated by thermodynamic measurement using tiny single crystal samples less than 10 μg . The materials we studied are $\kappa\text{-(BEDT-TTF)}_4\text{Hg}_{2.89}\text{Br}_8$ and $\kappa\text{-(BEDT-TTF)}_4\text{Hg}_{2.78}\text{Cl}_8$, where BEDT-TTF denotes bis(ethylenedithio)tetrathiafulvalene. These compounds are known to have non-stoichiometry concentrations and therefore incommensurate structure of donor layers and counter anion layers. The donor arrangement in the BEDT-TTF layer is the same as well known $\kappa\text{-(BEDT-TTF)}_2\text{X}$ (X: monovalent counter anion) which are known as a dimer-Mott triangular system that can make quantum spin liquid state [1, 2]. The non-stoichiometry composition yields 11% and 22% doping of hole carriers in the π -electrons layer.

The $\kappa\text{-(BEDT-TTF)}_4\text{Hg}_{2.89}\text{Br}_8$ shows a superconductivity while keeping the spin liquid like character in its temperature dependence of the magnetic susceptibility. Although the superconductive transition has been observed by heat capacity measurements around 3 – 4 K with a rather broad $C_p T^{-1}$ anomaly, its low temperature heat capacity has a quadratic term due to the nodal gap as in the other κ -type dimer-Mott superconductors. However, the fluctuation region above T_c is rather large and the normal state electronic heat capacity obtained by applying magnetic fields gives give large γ term of about 50 $\text{mJK}^{-2}\text{mol}^{-1}$ due to extraordinarily large electron correlations. The γ term of $\kappa\text{-(BEDT-TTF)}_4\text{Hg}_{2.78}\text{Cl}_8$ is also exceeds 50 $\text{mJK}^{-2}\text{mol}^{-1}$ probably the highest class among organic conductors and superconductors [1]. We discuss the origin of these anomalous features in doped spin liquid state in terms of non-Fermi liquid occurs in a kind of charge confinement effect in the dimer-unit in donor layers occurs in genuine Mott transition without accompanying any long-range magnetic ordering [2].

[1] S. Imajo, *et al.*, Phys. Rev. Res. 3 (2021) 033026.

[2] S. Yamashita, *et al.*, Low Temp. Phys. 50 (2024) 1-7.

CONTRIBUTED TALK, THU./16:25



PLX4720: new perspectives in an anticancer drug

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Targeted therapy has revolutionized the treatment of late stages melanoma, a cancer responsible for most part of skin cancer-related deaths. Its working principle consists in using a molecule to inhibit $BRAF^{V600E}$, the enzyme responsible for melanoma proliferation. The first molecule discovered able to inhibit $BRAF^{V600E}$ is PLX4720, an imidazole-based drug, also used in the treatment of other cancers where $BRAF^{V600E}$ plays a crucial role [1]. Unluckily, the low aqueous solubility of PLX4720 hinders medical applications. The knowledge of crystalline structure, crystallization properties and physical stability can help solve the problem, because the physical state, i.e. crystalline or amorphous, highly impacts on the bioavailability and dissolution rate of a generic pharmaceutical. Similar issues arise also in the glassy state whose practical application, favored by a higher dissolution rate, is hampered by metastability [2]. Finally, the presence of polymorphism, i.e. a molecule ability to stably arrange in various geometries, can play an important role. Surprisingly, despite the remarkable amount of clinical research, nothing has been done to characterize structural and physical properties of PLX4720.

In this work we employ Electron Diffraction, Differential Scanning Calorimetry (DSC) and Fast DSC (FDSC) [3] to study PLX4720 physical properties. DSC gives information about crystallization properties of PLX4720, discovering a second polymorph. Electron Diffraction has been used to characterize the crystalline structures of the original and the new polymorphs. Further knowledge of the crystallization properties of PLX4720 comes from FDSC, which has allowed us to find a third polymorph and to understand the real importance of thermal history on PLX4720 crystallization process.

[1] P. N. Ibrahim *et al.*, *Annu. Rep. Med. Chem.*, 45 (2013) 435

[2] W. Tu *et al.*, *J. Chem. Phys.*, 144 (2016) 174502

[3] D. Sonaglioni *et al.*, *Thermochim. Acta*, 719 (2023) 179385

POSTER SESSION

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- Juliusz C. Chojenka** (Kraków, Poland)
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- Magdalena Fitta** (Kraków, Poland)
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32. Metal-to-metal electron transfer in a bistable molecular chain magnet probed by X-ray absorption spectroscopy p. 100
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33. Improvement of prostate cancer contrast in MRI using core/shell nanoparticles and 9.4T MRI system p. 101
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POSTER NO. 1

Contrast enhancement in MRI using combined double action contrast agents and image post-processing in the breast cancer model

D. MacDonald¹, F. C. J. M. van Veggel², B. Tomanek^{1,3,4}, and B. Blasiak¹

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Gadolinium (Gd) and iron (Fe) based contrast agents, which reduce T_1 and T_2 relaxation times respectively, are frequently employed in MRI to enhance cancer detection. Recently, contrast agents that alter both T_1 and T_2 times, utilizing core/shell nanoparticles, have been developed. While the benefits of these T_1/T_2 agents have been demonstrated, the contrast in MR images between cancerous and adjacent normal tissues resulting from these agents has not been thoroughly examined. Previous studies focused on changes in cancer MR signal or signal-to-noise ratio post-contrast injection, rather than on the differences in signal between cancerous and adjacent normal tissues. Additionally, the potential advantages of T_1/T_2 contrast agents through image manipulation techniques such as subtraction or addition have yet to be fully explored. To address this, we conducted theoretical calculations of MR signals in a tumor model using T_1 -weighted, T_2 -weighted, and combined images for T_1 -, T_2 -, and T_1/T_2 -targeted contrast agents. These theoretical findings were complemented by in vivo experiments using core/shell $NaDyF_4/NaGdF_4$ nanoparticles as a T_1/T_2 non-targeted contrast agent in an animal model of triple-negative breast cancer. The results indicate that subtracting T_2 -weighted from T_1 -weighted MR images significantly enhances tumor contrast, with over a two-fold increase in the tumor model and a 12% improvement in the in vivo experiment.

POSTER NO. 2

Electronic and magnetic properties of infinite-layer nickelates

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The discovery of unconventional superconductivity in thin film nickelates marks a significant milestone in the field of high-Tc superconductivity. Similar to cuprates, infinite-layer nickelates feature planar NiO₂ layers containing 3d electrons from nickel, making them compelling subjects for study. Superconductivity has been confirmed exclusively in 20% hole-doped thin films [1, 2], indicating that both doping and interface play crucial roles in understanding this phenomenon. Therefore, we conducted a comprehensive DFT+U study on bulk NdNiO₂ and NdNiO₂/SrTiO₃ thin films to uncover their electronic and magnetic properties. We investigate how Sr doping influences the electronic and magnetic structures, with particular emphasis on the impact of 4f electrons from Nd. For thin films, we analyze both capped and uncapped multilayers, and utilize layer-projected density of states to elucidate the role of interfaces. Our findings reveal significant differences between thin film and bulk material, suggesting a complex interplay of interface effects, hole doping, and correlation physics in nickelate compounds.

[1] D. Li *et al.*, Nature, 572 (2019) 624

[2] S. Zeng *et al.*, Phys. Rev. Lett., 125 (2020) 147003

POSTER NO. 3

Influence of oxygen atom presence on twist-bend nematic phase in mixtures of CB7CB with alkoxy cyanobiphenyls

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Twist-bend nematic phase (N_{TB}) was known since 2011 [1]. High melting points of compounds forming this phase causes that it is monotropic (it exists below melting point). Because of that there are problems with examination of N_{TB} phase. Preparation of mixtures is one of method to lower melting points. But only in few papers miscibility studies of binary mixtures in which only one of compound forms N_{TB} phase was studied [2–4].

The aim of this work is the determination of the influence of oxygen atom in alkoxy chain cyanobiphenyls on temperature and concentration range of existing the N_{TB} phase in comparison to mixtures with alkyl cyanobiphenyls containing the same number of atoms in spacer between cyanobiphenyl groups. The presence of oxygen atom causes slightly increase of N_{TB} – N transition temperature.

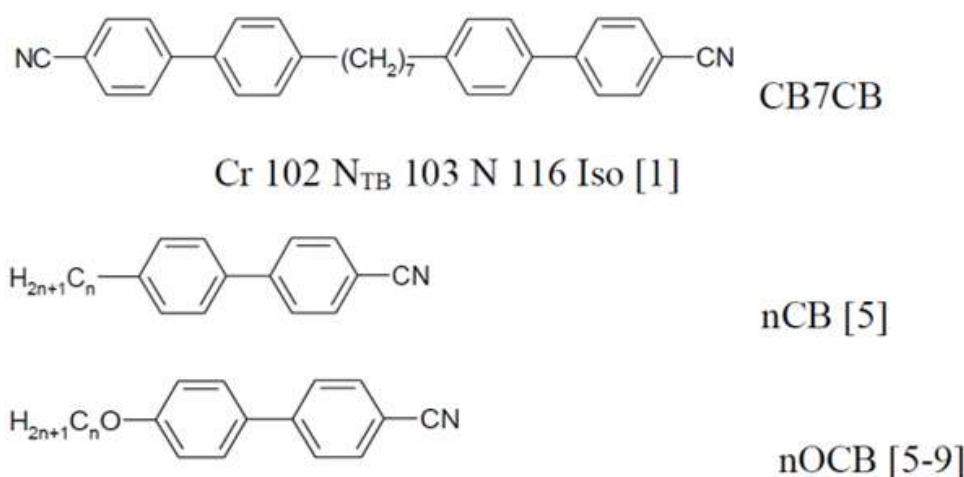


Figure 1: Structure tested compounds [1, 5–9].

- [1] M. Cestari *et al.*, Phys. Rev E, 84 (2011) 031704
- [2] Z. Lu *et al.*, Liq. Cryst., 41 (2014) 471
- [3] P. Oswald *et al.*, Phys. Rev. E, 105 (2022) 024707
- [4] M. R. Tuchband *et al.*, arXiv:1511.07523 (2015)
- [5] G. W. Gray *et al.*, Liq. Cryst. Ordered Fluids, 2 (1973) 617
- [6] G. W. Gray *et al.*, J. Chem. Soc. Perkin Trans II (1976) 97
- [7] P. Gorria *et al.*, Mol. Cryst. Liq. Cryst., 330 (1999) 175
- [8] G. W. Gray *et al.*, Ann. Phys., 3 (1978) 123
- [9] G. W. Gray *et al.*, J. Phys. Suppl., 36 (1975) 337

POSTER NO. 4

Magnetization reversal mechanism observed in FeCoNi nanowires

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Nanowires (NWs) are one-dimensional nanostructures with lengths of a few micrometers and diameters of the order of nanometers. Especially, magnetic nanowires with strong effective magnetic anisotropy are promising materials for 3D magnetic recording media technology due to their ability to smoothly propagate the domain wall at very high speed.

One of the most popular nanowire production methods is the template-assisted electrodeposition process, which enables obtaining NWs with the desired geometry, composition, and structure.

In this study, alloyed FeCoNi nanowires with three different diameters (40, 100 and 120 nm) and lengths of 6 μm were prepared within polycarbonate membranes. SEM images showed continuous NWs with smooth surfaces and constant diameters. The X-ray diffraction measurements revealed a polycrystalline *fcc* structure of FeCoNi. All nanowires exhibited magnetic anisotropy with an easy axis of magnetization along the nanowire axis. When the applied field was along the wire axis, the nanowire array exhibited rectangular hysteresis loops. For a field applied perpendicular to the wire axis, loops with similar coercivity but much smaller squareness were obtained. The angular dependence of the coercivity provides information about the magnetization reversal mode, which may be driven by two mechanisms: coherent rotation and curling magnetization. As the field orientation increased from $\theta = 0^\circ$, an increase in coercivity with a peak at $\theta = 70^\circ$ was observed for all samples. For $\theta \geq 70^\circ$ the coercivity decreased to reach a minimum along the hard axis ($\theta = 90^\circ$). This dependence may be explained by a combination of both coherent rotation and curling mode of the magnetization reversal process.

Acknowledgements: This research was supported by a French Government Scholarship.

POSTER NO. 5

Molecular dynamics simulations of the structure of amorphous pharmaceutical – probucol

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Amorphous-like pharmaceuticals have recently gained a lot of interest since they exhibit better solubility and bio-availability compared to their crystalline counterparts commonly used in tablet forms. Usually, such amorphous forms of active pharmaceutical ingredients (APIs) are produced by vitrification of melt. However, the variation in the melting temperature, cooling rate as well as applying mechanical milling or compression may affect their atomic-scale structure and related properties important from the application point of view [1, 2]. Therefore, understanding of basic correlations between the preparation process, structure, and properties is a prerequisite for further development of the amorphous pharmaceutical technology and their commercialization.

Due to very limited possibility of interpretation of subtle differences in the structure of various amorphous-like phases using standard characterization methods such as X-ray diffraction, usage of computer simulations is highly desired for verification of experimental data and obtaining of structural features difficult to extract based on solely of experimental data.

Here, Gromacs software was used to perform molecular dynamics simulations of the system of probucol API – is an anti-hyperlipidemic drug, at various temperature and pressure conditions in order to understand the changes into the intra- and inter-molecular structure induced by cooling and compression. The analysis of the total and partial structure factors, radial distribution functions, hydrogen bonds and molecular conformations allowed us to recognize differences in the structure between glasses produced by standard vitrification and the so-called “pressure-densification” method.

Acknowledgements: The authors acknowledge financial support from the National Science Centre, grant number 2021/41/B/NZ7/01654

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POSTER NO. 6

The interplay between thermal history and pressure and volume changes on the non-equilibrium behavior of polymers

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Literature data indicate that the various deviations from bulk behavior observed for polymers under nanoconfinement exhibit out-of-equilibrium features and can be eliminated through prolonged annealing. The time needed to recover the equilibrium state primarily depends on factors such as temperature, pore size, and the polymer's chain length [1–3]. In this presentation, we will discuss the influence of pressure and volume changes on the non-equilibrium glassy dynamics of poly(phenylmethyl siloxane) (PMPS 2.5k) confined within AAO nanopores. To explore this, we have conducted time-dependent measurements at the annealing temperature, following intermediate temperature jumps from higher (“down jump”) or lower (“up jump”) temperatures. Figure 1 illustrates the segmental relaxation times for PMPS 2.5k confined in 60 nm nanopores at the initial and final stages of annealing after up and down jumps. Our findings indicate that pore size, equilibration temperature, and depth jumps significantly influence the time required for the confined polymer to recover the segmental relaxation of the bulk sample. We have also shown that volume and pressure changes are closely linked with the equilibration process. After the down jump, the polymer needs to eliminate excess free volume to regain its bulk properties. Conversely, under up-jump conditions, the system gains volume during the annealing process, accompanied by corresponding pressure changes. Our study provides new arguments that the equilibration kinetics under nanopore-containment is related to volume and pressure changes.

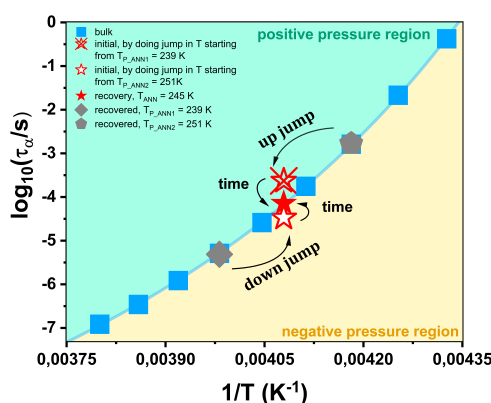


Figure 1: The segmental relaxation time vs inverse of temperature for PMPS 2.5k in bulk and confined in 60 nm nanopores. Data for confined samples were recorded under up- and down-jump conditions in the annealing temperature $T_{ANN} = 245$ K.

Acknowledgements: K. Chat is grateful for the financial support from the National Science Centre, Poland within the Project SONATINA 7 (dec. no. 2023/48/C/ST3/00179).

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POSTER NO. 7

Investigation of phase behaviour and selective light reflection in mixtures with azo compounds

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The multitude of existing and potential applications of liquid crystal materials highlights the crucial role of research on mesogenic multi-component systems. It makes it possible to design and predict the physicochemical properties of mixtures consisting of appropriately selected substances for which the phase sequence and phase transition temperatures are known. Detailed research using several experimental methods allows us to learn new ways of organizing molecules and observe the appearance or disappearance of certain mesophases and their stabilization in mixtures. Liquid-crystal thermography is one of the application examples, where selective light reflection can depend on the proportions of the mixture ingredients [1].

In this work, several two-component mixtures were prepared, containing various concentrations of individual components. The first component belongs to the mesogenic azo compound from the group of (E)-4-((4-alkoxyphenyl)diazenyl)phenyl alkanoates (nOABOOCm, for n = 3,5,7,8,10 and m = 1-19), e.g., 3OABOOCm [2]. The second one is a chiral liquid-crystalline compound from the group of cholesteryl derivatives (e.g., cholesteryl pelargonate) or chiral azobenzene derivative (e.g., (E)-4-((4-undecylphenyl)diazenyl)phenyl 2-chloropropionate [3]).

Polarized Optical Microscopy (POM) and Differential Scanning Calorimetry (DSC) methods were used to determine the phase transition temperatures and thermal properties of such mixtures. On their basis, phase diagrams were prepared, for which an analysis of changes in the phase behaviour with changes in composition will be presented. The work also concerns selective light reflection investigation of mixtures using the POM method.

Acknowledgements: MP has been partly supported by the EU Project POWR.03.02.00-00-I004/16.

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POSTER NO. 8

Self-assembly behavior of difluoroterphenyl derivatives differing with the linking bridge type

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The self-assembly behaviour and crystallization kinetics of two liquid crystal compounds, each featuring a 2',3'-difluorosubstituted terphenyl mesogenic core, have been detailed [1]. Calorimetric studies indicate that the type of linking bridge influences the polymorphism of smectic phases. The CH2O.3 compound [2], which has a $-\text{CH}_2\text{O}-$ linking bridge paired with a longer methylene spacer, exhibits a chiral smectic phase with antiferroelectric properties (SmC_A^* phase). In contrast, the COO.6 liquid crystal [3], with a $-\text{COO}-$ linking bridge and a shorter alkyl chain, forms a chiral smectic phase with ferroelectric properties (SmC^* phase). Both compounds undergo crystallization upon slow cooling, while fast cooling results in the vitrification of a conformationally disordered crystal phase. Dielectric measurements indicate complex relaxation dynamics in the identified thermodynamic states, and DFT calculations help estimate the nature of these relaxation processes.

The discovered findings could be highly significant for future research into liquid crystals and their potential applications. However, further investigation is needed to explore the relationships between mesophase organization and the phenomena of crystallization and vitrification, as well as their crystallization kinetics.

Acknowledgements: The PL-Grid Infrastructure and the ACC Cyfronet AGH (Krakow, Poland) are acknowledged for computational resources.

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POSTER NO. 9

First-principles investigations of structural, electronic, optical, and thermoelectric properties of ternary chalcopyrite semiconductor CuInTe_2

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The copper-indium-telluride chalcopyrite semiconductor CuInTe_2 has garnered significant attention due to its suitable bandgap for solar cells and high-temperature thermoelectric applications. In this study, we investigate the structural, electronic, optical, and thermoelectric properties of CuInTe_2 using state-of-the-art density functional theory (DFT) with the modified Becke-Johnson (mBJ) semilocal exchange functional. Our band structure calculations reveals that this compound exhibit a p -type semiconductors character with a direct band gap at the Γ point. The calculated band gap is in good agreement with the experimental data. Density of state analysis shows that this compound is primarily influenced by Cu d -states at the upper valence band and their hybridization with Te p -states bellow the first valence band. Furthermore, we validate our results by calculating optical properties, including the dielectric function, absorption coefficient, the real part of optical conductivity, optical reflectivity, and the refractive index. The refractive index finding shows reasonable agreement with the experimental data. These findings indicate that CuInTe_2 compound exhibits high absorption ($\approx 10^5 \text{ cm}^{-1}$) in the visible light range. Additionally, the Boltzmann transport theory was employed to analyze the thermoelectric properties. The calculation of Seebeck coefficient confirms the p -type nature of this compound. We found that the CuInTe_2 compound possesses a high electrical conductivity, and Seebeck coefficient with low thermal conductivity. According to our results, the figure of merit ZT can reach 1.66 at $T=1300 \text{ K}$ and for doping concentration of $1 \times 10^{20} \text{ cm}^{-3}$. This structure, with its suitable bandgap, is capable of absorbing a significant amount of light, making it a prospective choice for solar cells as well as for high-temperature thermoelectric applications.

POSTER NO. 10

The influence of the substrate on the properties of composite nanomaterials containing Mn₁₂-st single-molecule magnets

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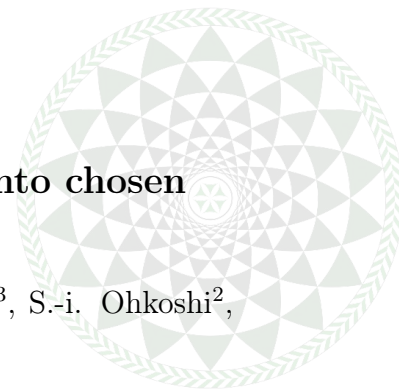
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The unique properties of Mn₁₂ single-molecule magnets (SMMs) make them promising candidates for applications in quantum computing, high-density data storage, and molecular electronics. However, the performance and stability of these SMMs are significantly influenced by the characteristics of the substrates on which they are deposited [1]. Our study investigates the effects of different types of substrates analyzing the substrate curvature and electrical conductivity on the properties of composite nanomaterials composed of Mn₁₂ stearate analogs (Mn₁₂-st) deposited on spherical carbon and silica nanoparticles. The Stöber method [2] was employed to obtain 150 nm and 300 nm diameter SiO₂ nanospheres, and the hydrothermal (HTC) approach [3] was adapted to synthesize 300 nm diameter carbon nanospheres. The magnetic molecules were linked to each kind of substrate via functional -COOH groups. All of the final products were characterized using several experimental techniques. We present hereby the results of electron microscopy (TEM and SEM), Fourier transform infrared (FT-IR) and Raman spectroscopy, energy dispersive X-ray spectrometry (EDS) and superconducting quantum interference device (SQUID) magnetometry. The experimental outcomes were brought together and compared to draw conclusions about the impact of the substrate's curvature, size and electrical conductivity on the characteristics and magnetic performance of our composite nanomaterials. These findings may prove beneficial for the future applications and magnetic nanomaterials development.

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POSTER NO. 11



An effect of small Au nanoparticle concentrations onto chosen properties in liquid crystal exhibits SmC_A^* phase

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A very simple and cheap way to obtain new liquid crystalline materials is to introduce nanoparticles (NPs) into the liquid crystal matrix. In our studies we used well-known liquid crystal (S)-MHPOBC as a matrix and Au nanoparticles (0.2 and 0.5wt.%) as dopant to check how the nanomaterial affects the properties of the matrix [1]. (S)-MHPOBC exhibits rich polymorphism and antiferroelectric phase SmC_A^* in a wide temperature range, therefore the research focused on the SmC_A^* phase. It was found that NPs do not influence liquid crystalline phases, however they are responsible for new crystal phases at concentration 0.5wt.%. The molecular reorientation time τ depends on the NPs concentration, which is related to the modified local electric field very close to the nanoparticle surface. In turn, the tilt angle θ is bigger only for concentration 0.5 wt.% Au NPs. The spontaneous polarization P_S is higher for both concentration which is associated to localized surface plasmonic resonance. The mentioned resonance is responsible for the induction of an electric dipole moment in the nanoparticle in the visible range, which in turn generates a strong electric field in its vicinity. The induced additional dipole moment contributes to the macroscopic polarization and the organic molecules surrounding the NPs experience a stronger electric field. The smectic layer distance D as well as the correlation length ξ is not affected by Au NPs. In the same time, the helical pitch p is increased in comparison to pure matrix and it decreases with decreasing temperature. Additionally, the influence of Au NPs on localization of absorption bands, electric permittivity, specific electric conductivity and relaxation processes will be presented.

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POSTER NO. 12

The presence of the phonon bottleneck and Raman process in magnetic relaxation of $\text{GdCl}_3 \cdot 6\text{H}_2\text{O}$

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Static and dynamic magnetic response of $\text{GdCl}_3 \cdot 6\text{H}_2\text{O}$ has been studied. Its crystal structure is ionic, with Gd(III) central atom exhibiting octa-coordination with O_6Cl_2 donor set. The two chloride ligands are in the close neighborhood. Based on the static magnetic susceptibility analysis, the effective moment was calculated yielding 7.88 emuK/mol, and the susceptibility analysis using Curie-Weiss law suggested the values of parameters $C = 7.824$ and $\theta = -0.08$ K. Weak magnetic coupling and/or single-ion anisotropy was confirmed by good agreement of magnetic field dependence of the magnetization and Brillouin function for $S=7/2$ system.

Two relaxation processes were identified during the study of alternating susceptibility. Slow relaxation was characterized by $\tau \sim T^{-n}$ dependence with $n_S = 2.31 \pm 0.04$ suggesting a strong role of phonon bottleneck effect. The structure enables to anticipate resonant phonon trapping as its potential source. The same type of dependence was found for the fast relaxation with $n_F = 3.23 \pm 0.09$. The anomalous value of n_F is close to theoretical predictions arising from assuming the combination effect of standard Raman relaxation mechanism and the interaction of magnetic ions with the local modes [1]. The existence of a standard Raman process was supported by the value of Debye temperature $\theta_D = 96.4$ K, obtained from specific heat studies, which significantly exceeds the energy level differences of Gd(III) ion. The simulation of molecular dynamics in $\text{GdCl}_3 \cdot 6\text{H}_2\text{O}$ revealed, the presence of a set of low-energy vibrational modes below 100 cm^{-1} supporting the scenario theoretically proposed in [1].

Acknowledgements: The work was supported by the Slovak grant agency APVV-22-0172.

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POSTER NO. 13

Exploring magnetocaloric effect of coordination polymer $\text{Mn}_2^{\text{II}}(\text{imH})_2(\text{H}_2\text{O})_4[\text{Nb}^{\text{IV}}(\text{CN})_8]\cdot 4\text{H}_2\text{O}_n$ by relaxation calorimetry

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Magnetocaloric properties of $\text{Mn}_2^{\text{II}}(\text{imH})_2(\text{H}_2\text{O})_4[\text{Nb}^{\text{IV}}(\text{CN})_8]\cdot 4\text{H}_2\text{O}_n$ molecular magnet are reported [1]. The coordination polymer crystallizes in the monoclinic $P2_1/c$ space group and displays a magnetic second-order phase transition at $T_c \approx 24.1$ K. The relaxation calorimetry measurements are analyzed in order to determine the temperature dependence of the magnetic entropy change ΔS_M as well as the adiabatic temperature change ΔT_{ad} for an array of applied field changes ranging from 0 to 9 T. For $\mu_0\Delta H = 5$ T the entropy change ΔS_M attains the maximum value of $6.55 \text{ J K}^{-1} \text{ mol}^{-1}$ ($9.5 \text{ J K}^{-1} \text{ kg}^{-1}$) at 25.5 K, while the corresponding maximum value of ΔT_{ad} amounts to 2.02 K at 25.1 K. The critical behavior of the isothermal entropy change is discussed. In particular, the analysis of the field dependence of ΔS_M in terms of the power law implies that the studied compound belongs to the mean-field universality class.

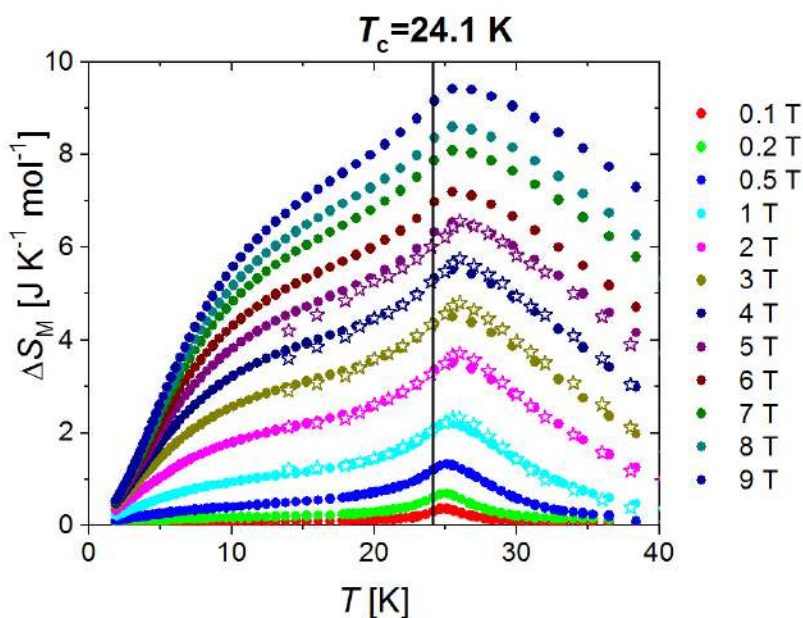


Figure 1: The isothermal entropy change ΔS_M for indicated magnetic field change values as a function of temperature. Apart from the values derived here (full symbols) shown are the values previously obtained using magnetometric methods (open stars) [2].

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POSTER NO. 14



Majorana bound states in superconducting ladder

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Majorana bound states can appear on the ends of a one dimensional chain due to the interplay between s-wave superconductivity, spin-orbit coupling and external magnetic field. Recent experimental progress has given unprecedented control over atoms and made it possible to build a chain via atom-by-atom engineering. The magnetic order of these atoms can also be controlled in the process creating an anti ferromagnetic order as observed in BaFe_2Se_3 . In this talk we will present our recent work, where we studied one such case where two chains are placed side by side forming a ladder like in BaFe_2Se_3 . Employing the tight binding model and symmetry arguments we categorize our system to be of BDI topological class assuming the periodic boundary conditions. We show various aspects of the topological phase from the evaluated winding number. We demonstrate the band inversion as the topological phase of the Ladder changes. To exemplify the presence of Majorana bound states, we study the ladder with finite size within the tight binding framework in real space. Evaluating the local density of states for the zero modes, we show the existence of Majorana fermions.

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POSTER NO. 15

Local structure of plasma-modified Mn(II)-Nb(IV) molecular magnet investigated with X-ray absorption spectroscopy

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Molecular magnets are promising materials for applications in modern technologies such as spintronics, magnetic refrigeration, and active sensors. A key challenge in this class of materials is obtaining systems with high enough Curie temperature T_C to effectively utilize their properties at a reasonable temperature range. The primary approach of the molecular magnetism community is to engineer materials at the molecular level by selecting appropriate synthetic building blocks and procedures. Another method is plasma treatment, a cost-effective and fast technique successfully used to alter the net magnetic moment, magnetic hysteresis loop, and T_C in ceramics, thin films, and nanoparticles. Despite promising prospects, plasma irradiation was never used in molecular magnets.

To address this research gap, we studied how plasma irradiation affects the magnetic properties of $[\text{Mn}^{II}(\text{H}_2\text{O})_2]_2[\text{Nb}^{IV}(\text{CN})_8] \cdot 4\text{H}_2\text{O}_n$ molecular magnet, which is known for its magnetocaloric effect and magnetic sponge behavior. Using plasma treatment, T_C raised by 20% from 49 K to 72 K. X-ray powder diffraction (XRD) confirmed the crystallographic structure remains unchanged, with a slight contraction of the unit cell that increased the superexchange coupling constants by 20%, as determined by the mean-field approximation.

The X-ray absorption near edge structure (XANES) for Nb L_2 - and L_3 -edges and extended X-ray absorption fine structure (EXAFS) analyses for the Mn K-edge were done to investigate how the local structures of the magnetic metal centers are affected by plasma irradiation. The results point to the shortening of the interatomic distances after plasma irradiation by 1-2%. Consequently, the first coordination shell is closer to Mn by approximately 0.02 Å, which confirms the qualitative conclusions drawn from the XRD. This leads to the modification of superexchange coupling constants that are sensitive to interatomic distances. The increase in T_C was probably related to the desorption of four or fewer molecules of H_2O of crystallization, while all four coordinated H_2O were maintained.

Our findings demonstrate that plasma-induced modifications in molecular systems are a quick, reliable, and effective way to obtain unique magnetic phases that would otherwise be unattainable. Such changes can then be investigated using synchrotron methods, generating fresh perspectives on achieving high- T_C systems for technological purposes.

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POSTER NO. 16

Analysis of the physical properties of the ZIF-67 and its diamagnetic analogue ZIF-8

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Zeolitic imidazolate framework (ZIF) materials represent metal–organic frameworks with three-dimensional porous structure formed by metal ions linked via imidazole linkers. This work is devoted to the study of $[\text{Co}(\text{mIm})_2\alpha]$, abbreviated as ZIF-67 and its diamagnetic analogue $[\text{Zn}(\text{mIm})_2\alpha]$ known as ZIF-8 ($\text{HmIm} = 2\text{-methylimidazole} = \text{C}_4\text{H}_6\text{N}_2$). The rapid synthesis in water produced nanocrystallites. XRD, infrared and Raman measurements confirmed that both compounds have identical crystal structure and vibration spectra with the only difference that Co atoms in ZIF-67 occupy the positions of Zn in ZIF-8.

The heat capacity of the powder samples was measured from 0.4 to 300 K in zero magnetic field. Magnetic specific heat of ZIF-67 was obtained by subtraction of ZIF-8 specific heat which can be treated as lattice contribution. The magnetic contribution C_{mag} is characterized by a round maximum at 11 K, typical for low-dimensional systems. Corresponding magnetic entropy agrees with the prediction for spin 3/2. The application of magnetic field had negligible effect on the round maximum. The magnetic susceptibility in 10 mT shows bifurcation of field cooling (FC) and zero field cooling (ZFC) data at 14 K but in 100 mT the splitting shifts to 5 K and finally it disappears completely in fields above 1 T. The application of Curie–Weiss law provides $g = 2.2$ and $\theta = -44$ K, reflecting moderate antiferromagnetic interactions. The isothermal magnetization $M(B)$ of ZIF-67 was measured at 0.46 K. At fields up to 1T, the $M(B)$ deviates from the linear dependence, which corresponds with the appearance of bifurcation of ZFC and FC data below 1 T. The character of magnetism in ZIF-67 is discussed.

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POSTER NO. 17

Mechanocaloric properties of polyurethane rubbers with different crosslink density

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Rubbers consist of crosslinked polymer chains, which can be orientationally ordered upon uniaxial stretching. As this ordering process causes the reduction of configurational entropy, rubber stretching under adiabatic condition results in a slight increase of temperature known as a mechanocaloric effect. The rubber elasticity consists not only of entropic contribution but also of energetic contribution because the interaction between the adjacent polymer chains can be changed by the rubber stretching. The contribution ratio of the two components depends on the polymer species, types of crosslink, and crosslink densities.

In this study, we investigated the thermodynamic origin of the elasticity for chemically crosslinked polyurethane rubbers. We synthesized three strips of rubbers with different crosslink density, and simultaneously measured the stress and temperature changes upon uniaxial stretching using a laboratory made calorimeter.

The mechanical energy (E_{mech}) applied to the rubber through the stretching was evaluated from the stress, and the thermal energy (E_{therm}) generated from the rubber was determined from the temperature changes. Both E_{mech} and E_{therm} increased with increasing crosslink density, and the E_{mech} and E_{therm} were found to be almost identical to each other (Fig. 1). This means that the internal energies of the rubbers do not change upon stretching, and the entropic contribution to the rubber elasticity is dominant irrespective of the crosslink density. The crosslink densities evaluated from the entropy changes were considerably greater than those calculated from the amount of crosslinkers used on the synthesis, which indicated that the hydrogen bonding between the polymer chain may act as additional crosslink spots.

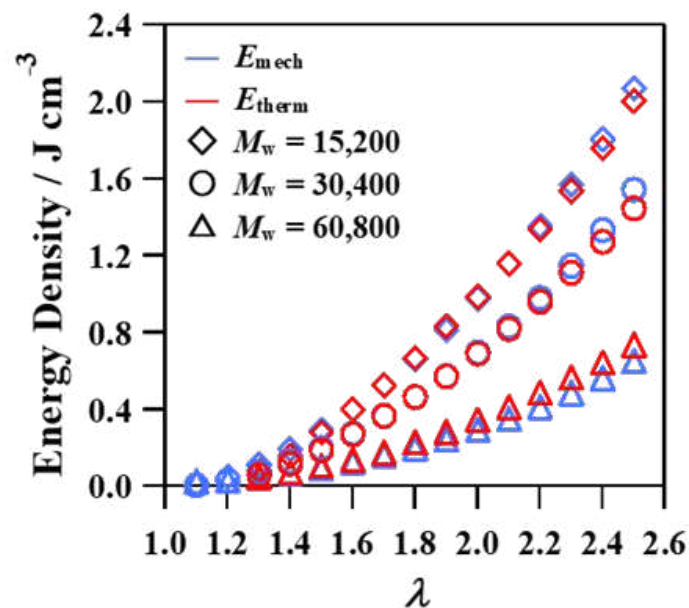


Figure 1: E_{mech} and E_{therm} of polyurethane rubbers with different crosslinking densities at different stretching ratios ($\lambda = l/l_0$) from 1.0 to 2.6. M_w s represent the averaged molecular weights between the two crosslinks.

POSTER NO. 18

Study of the structural properties-electrical resistivity relations of carbon spheres prepared by hydrothermal carbonization

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Graphitization of carbon materials influences their microstructure and conductivity, which in turn affects their applications. There are still few reports on studying the relationship between the structure and conductive properties of hydrothermal carbon spheres (CS) after graphitization.

This research focuses on the preparation of CS resulting from hydrothermal treatment using glucose as a precursor. The effects of temperature, synthesis time, and the addition of cetyltrimethylammonium bromide (CTAB) on the size and size distribution of CS as well as the process yield were determined. The results showed that particle size can be easily controlled by temperature and synthesis time. Additionally, by changing the concentration of the surfactant, we can influence the morphology and size dispersion of the spheres. The obtained carbon materials were characterized using scanning electron microscopy (SEM), Raman spectroscopy, thermogravimetric analysis (TGA), nitrogen adsorption analysis and resistance measurements.

To observe the effect of sphere size and its size distribution on their conductivity, three series of monodisperse (200, 300, and 400 nm) and polydisperse CS were investigated. They were subjected to thermal treatment at temperatures ranging from 600 to 1000°C in an N₂ atmosphere. These studies showed that their surface structure, microstructure, porosity, and polygonization strongly depend on the treatment temperature. We also investigated the resistivity of the particles as a function of their surface area, microstructure, density, and sphere size.

The results highlight the key role of synthesis parameters in adjusting the physical and electrical properties of carbon spheres, presenting valuable implications for their application in electronic devices.

POSTER NO. 19

The new family of photomagnetic coordination frameworks based on $[\text{Mo}(\text{CN})_7]^{4-}$ building blocks

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Polycyanometallates are well-known as building blocks for the construction of coordination frameworks which show magnetic or photomagnetic behavior and other effects such as SGH, luminescence, SCO, porosity, etc [1]. We recently discovered that potassium heptacyanomolybdate(III) can be an excellent precursor for designing photomagnetic systems due to its intrinsic spin state photoswitching behavior, high relaxation temperature of the photoexcited state and reverse photoswitchability after irradiation with a different wavelength [3]. During our ongoing research, four coordination systems based on manganese(II), imidazole and heptacyanomolybdate(III) were discovered and characterized structurally and magnetically. Their spectroscopic properties and photomagnetic behavior was also investigated [2]. All four compounds show long range magnetic ordering and it was discovered that upon 405 nm irradiation the magnetic ordering temperature (T_c) increases in each case. The underlying photoswitching mechanism is associated with the photodissociation of one of the cyanide ligands from the low-spin $[\text{Mo}(\text{CN})_7]^{4-}$ followed by the formation of a high spin $[\text{Mo}^{\text{III}}(\text{CN})_6]^{3-}$.

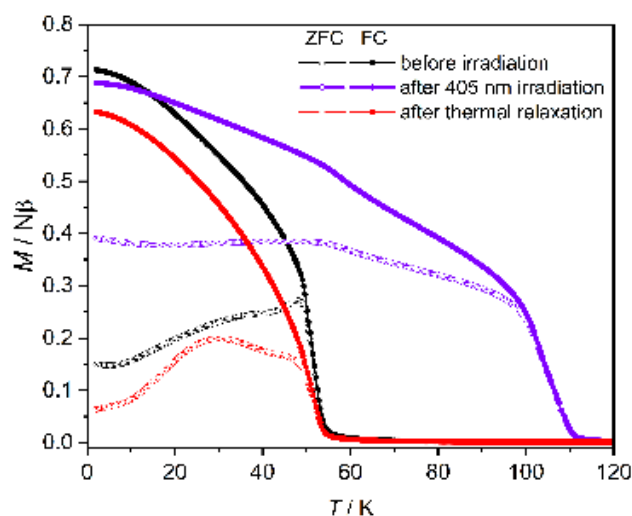


Figure 1: ZFC-FC curves at 50 Oe for the compound $[\text{Mn}^{\text{II}}(\text{imidazole})_2][\text{Mo}^{\text{III}}(\text{CN})_7]_n$ before and after irradiation with 405 nm light and after thermal relaxation at 350 K.

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- [3] manuscript in preparation

POSTER NO. 20

Domperidone co-amorphous phases with xanthine derivatives

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Most active pharmaceutical ingredients are delivered orally in crystalline solid forms, which often have poor aqueous solubility. Co-amorphization with small-molecule co-formers has been proposed as an alternative strategy to enhancing the kinetic stability of these high-energy, disordered states [1].

Domperidone (DPD) is a dopamine antagonist medication used for the treatment of nausea, vomiting, gastroparesis, and lactation enhancement. Its bioavailability is limited by poor water solubility. The formation of a co-amorphous system involving domperidone is here investigated, using several xanthine derivatives as small molecular co-formers. These were selected for their variety of H-bond donors and acceptors, interacting differently with DPD and potentially enhance its properties.

The co-amorphous systems were prepared by mechanochemistry and characterized using various analytical techniques. These included X-ray diffraction (PXRD), differential scanning calorimetry (DSC), and infrared spectroscopy (FTIR-ATR). Additionally, quantum chemistry calculations using density functional theory (DFT) and molecular electrostatic potentials (MEP) were used to elucidate the intermolecular interactions in the DPD co-amorphous systems.

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[1] J. F. C. Silva *et al.*, *Cryst. Growth Des.*, 23 (2023) 6679

POSTER NO. 21

Asymmetric magnetization reversal tailored by different oxidation procedures in Co/CoO exchange-biased thin films

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The exchange bias effect is a magnetic phenomenon associated with a unidirectional exchange anisotropy which appears at the interface between a ferromagnet and an antiferromagnet. Due to this coupling, the magnetization reversal in one field sweeping direction is more energetically demanding than in the other which leads to the shift of a magnetic hysteresis loop from the zero position known as the bias field H_{ex} . The exchange bias effect is sensitive to the condition of the interface between a ferromagnet and an antiferromagnet. Especially, its magnitude is dependent on the roughness of layers, intermixing of constituent materials, and structural order at the interface.

In this work, we report on the asymmetric magnetization reversal for the model CoO/Co exchange-biased system. The antiferromagnetic CoO layer was prepared in three different ways – natural oxidation in ambient conditions, oxidation in vacuum in partial oxygen pressure, and by plasma treatment. We focus on changes in magnetic properties induced by various procedures and combine them the condition of the antiferromagnetic-ferromagnetic interface studied by chemical depth profiling. The reversal along the upper hysteresis branch shows the wall motion while the switching along in opposite field direction indicates an influence of the coherent magnetization rotation. In all cases the hysteresis loops are asymmetrical and the asymmetry is dependent on the temperature and on the type of procedure used to obtain CoO layer (see Figure 1).

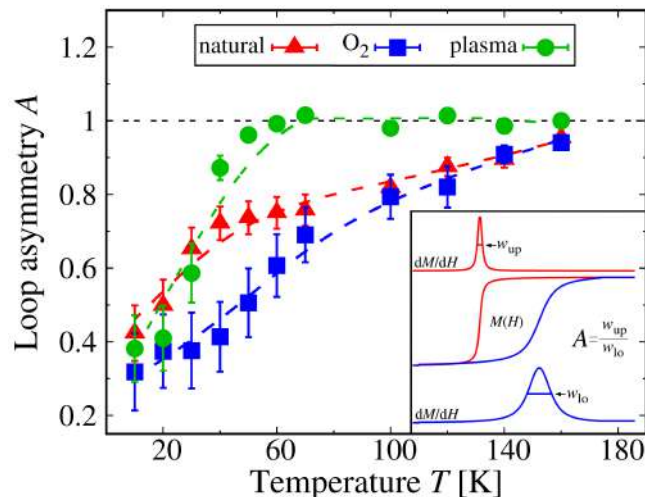


Figure 1: Magnetic hysteresis loop asymmetry parameter A calculated from the dM/dH switching field distributions measured for the natural, O_2 , and plasma samples. Dashed lines are a guide for the eye. The inset schematically shows the way the A parameter was determined.

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POSTER NO. 22

Pulsed laser induced solvent-nanoparticle chemo-physical interaction; an effective approach toward creation of submicron heterostructures

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Creating heterostructures has been a brilliant solution to address the increasing need for innovative materials in high-tech applications. Heterostructures possess distinct attributes that render them highly promising for the development of sustainable and environmentally friendly energy systems with a diverse range of applications across multiple fields, such as catalysis, energy storage, and solar energy harvesting. In this study, we aim to investigate a promising and innovative approach for producing heterostructures involving the use of pulsed laser irradiation on suspended nanoparticles. Our main focus lies in understanding the chemo-physical interactions that occur at the interface between the solvent and the nanoparticles when they are adjusted to the laser pulses. When the nanoparticles are exposed to the laser pulses, they absorb the energy from the pulses, causing the solvent molecules in contact with them to gain kinetic energy. This increase in energy is sufficient for the solvent molecules to dissociate and diffuse into the molten nanoparticle, leading to the formation of different phases [1]. The formation process involves both physical phase transitions and chemical oxidation/reduction reactions, which are highly influenced by the chemical environment and temperature of the reaction [2]. These variables were adjusted accordingly based on the suspension and laser parameters to achieve the desired heterostructures. An example of the formation of copper quantum dot on the surface of Fe₃O₄ using laser irradiation has been illustrated in Figure 1a. The particle growth mechanism is also depicted schematically in Figure 1b. Further exploration of the process by which phases were created is being studied through the application of atomistic modeling techniques. In this study, density functional theory (DFT) calculations were employed to determine the reactive bond force fields. These force fields are subsequently utilized to investigate the breaking and formation of bonds in the respective systems, employing molecular dynamics (MD) simulations.

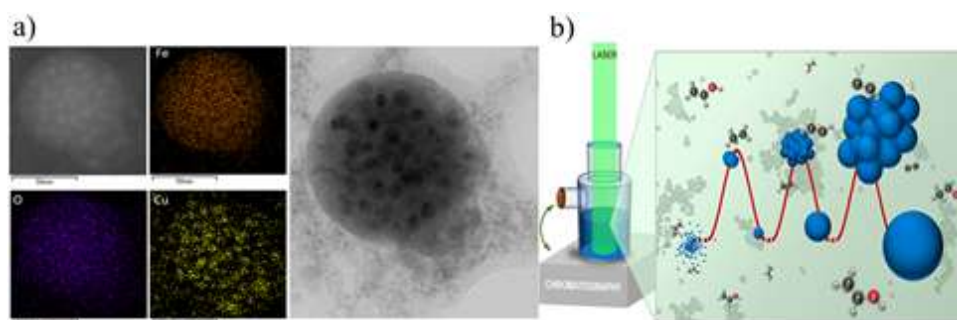


Figure 1: (a) Formation of copper quantum dot on magnetite nanoparticles, and (b) schematic of growth mechanism during pulsed laser irradiation of suspended nanoparticles.

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POSTER NO. 23

Unusual phase transformation kinetics in FePd thin films – intermediated phases and its magnetic properties

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In this study, we investigate the phase transformation process between Fe/Pd multilayer and L1₀ FePd alloy. The transformation is studied at different stages of post-deposition annealing to track the progress of chemical ordering and phase transformation. For that purpose, we combined SEM, XRD and Mossbauer spectroscopy techniques. It allowed to identify an unusual way of transformation through two parallel and competitive paths. The first one includes the stoichiometric route of A1 and A6 phases, and the second off-stoichiometric route with L1₂ and L1' phases. The process ends with the formation of the L1₀ phase. We found that one of the most important factors determining the type of phase transformation is solid state dewetting. When the dewetting progresses rapidly the change in the kinetic growth is observed from a low-dimensional to a three-dimensional growth mechanism that primarily affects the L1₀ phase formation [1].

Parallel to structural research, we study the changes in magnetism properties with the evolution of film morphology and phase composition. We found that the major changes are observed when the dewetting progresses and the film loses its continuity. Then the fast growth of the L1₀ phase happens influencing the magnetization reversal mechanism and yielding the magnetic spring-like behavior [2]. Since the solid state dewetting process influences the type of phase transformation and intermediated phases contribution, it creates new opportunities for using this phenomenon to tailor the magnetic properties of thin alloy films.

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POSTER NO. 24

The influence of technological conditions on the electrical conductivity and thermoelectric properties of sodium-bismuth titanate (NBT)

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The lead-based ceramic materials commonly used so far, such as PZT, should be replaced with lead-free materials due to the content of toxic elements. One of the materials that could replace lead-based materials was discovered by Smolensky et al. $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ (NBT) [1]. However, the piezoelectric properties of NBT are not as good as the piezoelectric properties of PZT [2, 3]. In order to improve the properties of NBT, solid solutions based on it are tested. Another way to improve the properties of NBT is to obtain this material under various sintering conditions.

The tested lead-free $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$ ceramics were prepared by the conventional solid-state reaction method and hot pressing method. Measurements of electrical conductivity (alternating current σ_{ac} and direct current σ_{dc} , Seebeck coefficient and determination of the linear coefficient of thermal expansion were aimed at examining the influence of sintering conditions on these properties. Conductivity measurements obtained for all tested samples indicate that the number of re-sintering or hot pressing affects the electrical conductivity values. The value of the obtained Seebeck coefficients and the value of the linear thermal expansion coefficients on individual samples also show that modification of the sintering process can improve or worsen the obtained values

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POSTER NO. 25

Liquid crystalline glassformer forming hexatic smectic X_A^* glass – DFT calculations for interpretation of X-ray diffraction and IR spectroscopy data

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The chiral mesogenic compound, abbreviated as 3F7HPhH6, forms on cooling four smectic phases: paraelectric SmA^* , ferroelectric SmC^* , antiferroelectric SmC_A^* and tilted hexatic SmX_A^* (SmF_A^* or SmI_A^*). SmX_A^* forms the glass below $T_g = 230$ - 233 K. During heating of the supercooled sample, one or two crystal phases (for 2 K/min or 5-20 K/min, respectively) are observed upon cold crystallization. The fragility index of this glassformer, determined from the α -relaxation time, is equal to 94.5 [1]. The tilt angle of molecules, measured by the electro-optic method, reaches 44° in the SmC_A^* phase [2]. By comparing the tilt angle with the smectic layer spacing, determined by X-ray diffraction, one can obtain the molecular length $L = 34 \text{ \AA}$ and shape parameter $\delta\Theta = 25^\circ$. The latter is an angle between two vectors: one connecting the terminal C and F atoms, and another describing the direction of the aromatic molecular core. The high $\delta\Theta$ value indicates that 3F7HPhH6 molecules have a strongly non-linear shape. DFT calculations performed in Gaussian 16 [3] allow us to find the molecular models with L , $\delta\Theta$ close to the experimental values. The models are subsequently used for the calculation of theoretical IR spectra and assignment of the vibrational modes to the experimental IR absorption bands.

Acknowledgements: We thank Assoc. Prof. Wojciech Zając (IFJ PAN) for help with DFT calculations, performed in Ares supercomputer from the Academic Computer Centre Cyfronet AGH (PLGrid Infrastructure).

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POSTER NO. 26

Nanogarnet quest: unveiling high-yield monocrystalline YIG nanoparticles

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Yttrium iron garnet (YIG, $\text{Y}_3\text{Fe}_5\text{O}_{12}$) is known for its exceptional magnetic and optical properties, making it a material of significant interest in various technological applications, including magnetic sensors and photonic crystals. Traditionally, the synthesis of YIG involves large single-crystal forms to ensure high purity and crystallinity. In contrast, our research focuses on the synthesis of YIG nanoparticles, which offer enhanced surface area while maintaining the desirable properties of bulk YIG crystals.

Our study presents a detailed methodology for synthesising YIG nanoparticles with high monocrystallinity. We provide an explicit recipe alongside a calculation of the reaction yield. Our method achieves a yield that approaches the theoretical maximum efficiency, indicating that nearly the entire precursor material is converted into the desired YIG product.

XRD and TEM electron diffraction confirm the single-phase nature and high monocrystallinity of the synthesised YIG, with the single-crystal size approximately 146 nm. TEM reveals a particle size of around 150 nm, indicating almost entirely single-crystal nanoparticles.

Magnetic properties were investigated using SQUID magnetometry. The synthesised nanoparticles retain high magnetic saturation and low coercivity, making them suitable for high-performance applications.

Potential applications include hyperthermia for cancer treatment and a far-reaching goal of utilising them in neural networks.

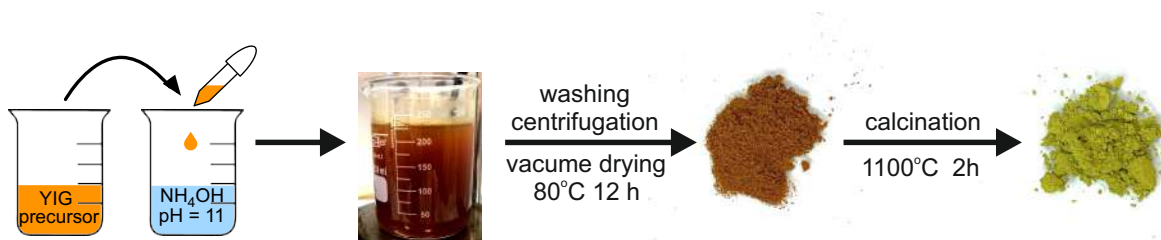


Figure 1: A schematic representation of the synthesis route.

POSTER NO. 27

Magnetism of $\text{NdMn}_{1-x}\text{Ti}_x\text{O}_3$ system

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We present the determination of structural stability of $\text{NdMn}_{1-x}\text{Ti}_x\text{O}_3$ ($0 \leq x \leq 0.4$) compounds and a subsequent study of the magnetic properties of the stable systems. Preparation using the float zone method in an air atmosphere is feasible without secondary phases for concentrations up to $x \leq 0.3$. Furthermore, the compounds exhibit long-term temperature stability at $T = 900^\circ\text{C}$ in an air atmosphere for $x \leq 0.3$ and short-term temperature stability up to 1100°C for $x \leq 0.2$. The heat treatment of the samples impacts their magnetic properties.

The magnetic ordering temperature (T_N) of as-prepared samples decreases with T_i substitution, starting from 85.1 K for $x = 0$, to 75.2(5) K for $x = 0.1$, 68.7(3) K for $x = 0.2$, and 38.4(2) K for $x = 0.3$. The zero-field-cooled (ZFC) magnetization curve of $x = 0.1$ sample exhibits a compensation point at $T_1 = 58.4$ K. The heat treatment (900°C , air atm., 48 h) significantly increases the oxygen content in the samples. T_N of annealed samples yields 84.2(2) K; 76.2(2) K; and 69.9(2) K for $x = 0$; $x = 0.1$ and $x = 0.2$. The $x = 0$ sample exhibits compensation point on ZFC curve at 7.4(2) K and 2 magnetic compensation points at 30.6 K and 58.2 K on the field-cooled (FC) curve. FC curve of $x = 0.1$ sample exhibits compensation points at 31.5(2) K and 43.1(2) K, but no compensation point was found on ZFC curves.

We conclude that the magnetism of $\text{NdMn}_{1-x}\text{Ti}_x\text{O}_3$ perovskite and other perovskite compounds strongly depends on the oxygen content in the samples. This is likely the key reason for the inconsistencies in the reported physical properties found in the literature. A more detailed analysis of this issue will be presented in the contribution.

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POSTER NO. 28

Controlling the photoactivity of nanopatterned titanium oxide

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The versatility of titanium dioxide lies in its intrinsic properties such as the wide bandgap between valence and conduction bands giving the possibility to generate electron-hole pairs, by irradiating it with sunlight, capable of inducing oxide-reduction reactions that are the fundamentals of the photocatalysis process. The photocatalytic properties of TiO₂ are dependent on the electronic and crystalline structure, specific surface area, morphologies, pore structure, and exposed surface facets. However, the catalytic performance of TiO₂ is strongly determined by the material surface, where the photoinduced reaction occurs, and photoexcited electrons and holes may migrate through this region. Therefore, the surface exposed to the light plays a crucial role in the photoactivity of titanium oxide. One of the most effective ways of maximizing the working surface area of the active material can be done by nanopatterning.

In this work, we show new approach to create highly ordered titanium oxide nanotubes by combining nanosphere lithography and anodization. The photoactivity of the TiO₂ nanotubes was studied by fluorescence spectroscopy in the UV-Vis range as a function of the patterning period and annealing temperature. The crystal structure of the nanotubes was characterized by X-Ray diffraction and Raman spectroscopy and compared to the material obtained by classical anodization. The fluorescence spectroscopy measurements revealed that the parameters of the patterning process have a strong influence on the photooxidation effect. These results indicate that the combination of pre-patterning and anodization provides an excellent tool for controlling their photoactivity.

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POSTER NO. 29

Positron annihilation studies of $\text{La}_{1-x}\text{Ag}_x\text{MnO}_3$ nanoparticles

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Magnetic nanoparticles $\text{La}_{0.70}\text{Ag}_{0.25}\text{MnO}_{3+\delta}$ (O2Ag25) and $\text{La}_{0.80}\text{Ag}_{0.15}\text{MnO}_{3+\delta}$ (O2Ag15) annealed at 800°C/48h in O₂ with the Curie temperature T_C of about 320 K and high value of the change of magnetic entropy $|\Delta S_{max}|(4T)$ of about 4 Jkg⁻¹K⁻¹ in the vicinity of T_C belongs to promising functional materials. Both samples crystallize in rhombohedral crystal structure (space group $R\bar{3}c$) with the volume of elementary cell of about 349 Å³. Thermogravimetric measurements (TGA) revealed huge mass drop at about 800°C which is connected with reduction of oxygen. Annealing in oxidative atmosphere up to 1400°C do not change the crystal structure but the volume of elementary cell increases to about 353 Å³ which may indicate presence of oxygen vacancies. Annealing in Ar up to 1400°C results in change of crystal structure, sample contains of about 80% new phase with orthorhombic crystal structure ($Pnma$). Both heat treatments lead to a drastic reduction of T_C and highlight the importance of oxygen content on magnetic properties. The aim of our paper is a spectroscopic study of the positron annihilation lifetime which provides information on the perturbations of the crystal structure caused by heat treatment. The main results of positron lifetime components (τ_i) and their relative intensities (I_i) are collected in the Table, the effect of annealing is eminent. In the contribution we will provide detail discussion of results with respect to X-ray powder diffraction, TGA and magnetization measurements.

SAMPLE	I ₁ (%)	τ_1 (ps)	I ₂ (%)	τ_2 (ps)	Mean lifetime (ps)
O2Ag15	74.7	166.2	25.3	345.3	211.5
O2Ag25	76.8	180.9	23.2	346.5	219.4
O2Ag15 annealed at 1400°C in air	28.2	180.0	71.8	290.0	259.7
O2Ag25 annealed at 1400°C in air	34.1	178.9	65.9	287.9	250.7
O2Ag25 annealed at 1400°C in Ar	51.5	178.0	48.5	305.9	240.0

Figure 1: Positron Annihilation Lifetime Spectroscopy - Results.

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POSTER NO. 30

Spin state switchability in Llrge coordination clusters

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The intensive development of technology creates a variety of challenges in the miniaturisation of physical systems dedicated to the detection of specific external stimuli as well as information storage/processing. In this context, one of the perfect candidates are molecular compounds with two or more inequivalent spin states, which could be switched by convenient external stimulus such as temperature, light, electric current or chemical activation.[1]

The presentation will focus on results considering synthesis and physicochemical properties of large undecanuclear coordination cluster $\{\text{Fe}^{II}[\text{Fe}^{II}(\text{bzbpn})]_6[\text{W}^V(\text{CN})_8]_2[\text{W}^{IV}(\text{CN})_8]_2 \cdot \text{solv}\}$, representing switchable magnetic properties realized via spin crossover (SCO) phenomena stimulated by temperature or sorption/desorption of solvent (fig 1).[2]

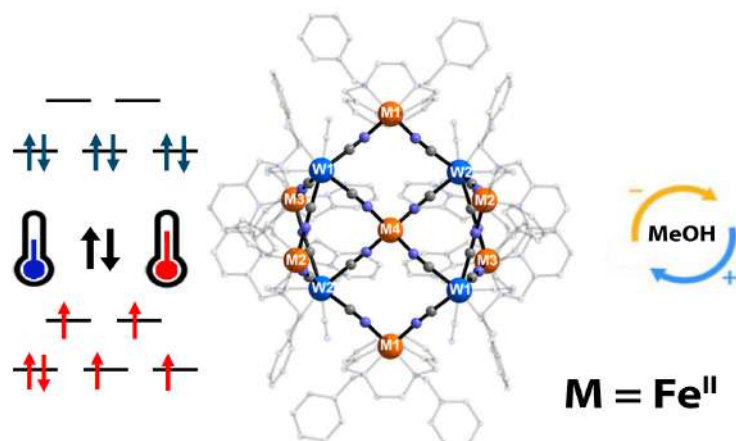


Figure 1: Coordination skeleton of $\{\text{Fe}^{II}[\text{Fe}^{II}(\text{bzbpn})]_6[\text{W}^V(\text{CN})_8]_2[\text{W}^{IV}(\text{CN})_8]_2 \cdot \text{solv}\}$ undecanuclear cluster.

Acknowledgements: We gratefully acknowledge National Science Centre (Poland) for financial support, project number UMO-2019/35/B/ST5/01481 and 2022/06/X/ST4/01277

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POSTER NO. 31

Novel 1,5,9-triazacoronene decorated with dioxothiadiazole units for multifunctional molecular materials

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Heterocyclic organic compounds with multiple heteroatoms such as nitrogen or sulfur are commonly studied in molecular science considering their various attractive properties. An interesting group of compounds are 1,2,5-thiadiazole 1,1-dioxides (dioxothiadiazoles) due to their electrochemical, luminescent, and magnetic features along with chemical and physical stability [1]. To improve their multiple properties novel dioxothiadiazole derivatives using 1,5,9-triazacoronene as a multifunctional core were proposed because of their strong fluorescence and excellent electron delocalization. Such redox-active compounds can be applied in organic electronics, solar panels, or light-emitting diodes [2]. Furthermore, presence of electron-poor pyridine rings makes them promising materials for *n*-type semiconductors [3]. In pursuit of this goal, a series of organic compounds was synthesized starting from 1,2-dimethoxybenzene.

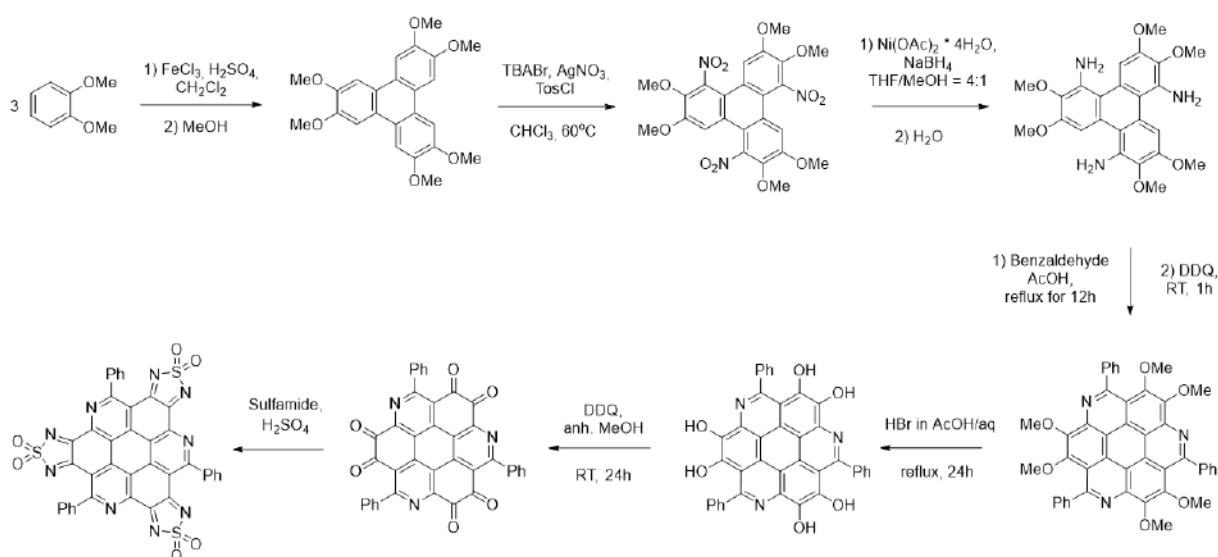


Figure 1: Reaction pathway to obtain compounds containing dioxothiadiazole units decorating the 1,5,9-triazacoronene core.

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- [1] P. Pakulski *et al.*, Chem, (2024)
- [2] M. Takase *et al.*, J. Am. Chem. Soc., 135, 21 (2013)
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POSTER NO. 32

Exploring the spin crossover transition in Fe(II)- triazole nanoparticles by X-ray absorption spectroscopy

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Spin crossover (SCO) complexes exhibit exceptional molecular bistability, allowing for reversible and controllable transitions between low-spin (LS) and high-spin (HS) states. This responsive behavior, combined with the ability to form nanoscale architectures, drives their wide-ranging applications in chemical sensing, switchable devices, displays, and data storage.

In this report, we investigate Fe(Htrz)₂(trz)@SiO₂ (Htrz: 1,2,4-triazole) nanoparticles of varying sizes (42±9 × 21±5 nm and 113±19 × 53±15 nm), synthesized using a reverse micelles method with the non-ionic surfactant Triton X-100. The particles were further coated with a silica shell via tetraethyl orthosilicate (TEOS). Structural changes during the SCO transition were examined using X-ray absorption near-edge structure (XANES) at the Fe K-edge. The most significant increase in absorption during the LS to HS transition correlates with the increased Fe-N bond distance, highlighting the established relationship between edge absorption intensity and bond distance.

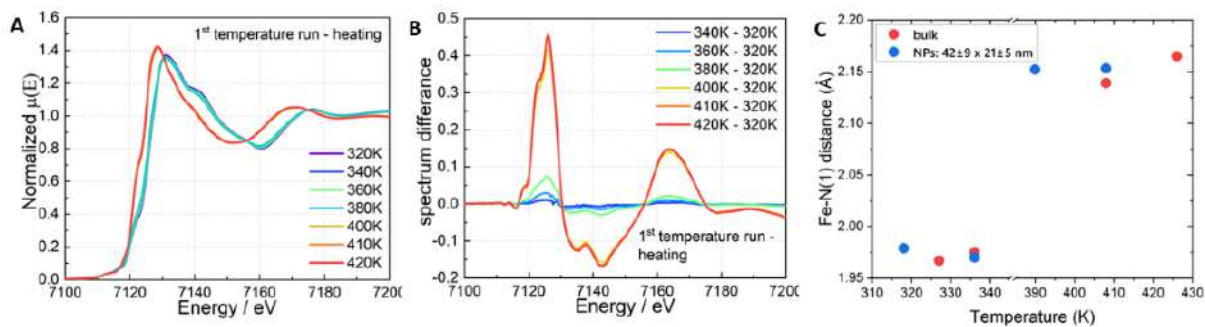


Figure 1: Fe K-edge XANES spectrum of the [Fe(Htrz)₂(trz)](BF₄)@SiO₂ nanoparticles (size 42±9 × 21±5 nm) collected at various temperatures (A). The difference between X-ray absorption of the high-spin and low-spin of the [Fe(Htrz)₂(trz)](BF₄)@SiO₂ nanoparticles (B). The average first Fe-N distance as a function of temperature calculated for NPs and bulk samples

POSTER NO. 33

Metal-to-metal electron transfer in a bistable molecular chain magnet probed by X-ray absorption spectroscopy

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Metal-to-metal charge transfer (MMCT) entails electron transfer between metal ions, creating valence isomers with different electronic configurations. This process alters spin states, coupling interactions, and charge distribution, significantly impacting the material's magnetic, electric, and optical properties, as well as bond lengths and thermal behavior.

In this report, we present the investigation of redox states in the CN-bridged coordination chain $\text{NH}_4[\text{Ni}(\text{cyclam})][\text{Fe}(\text{CN})_6] \cdot 5\text{H}_2\text{O}_n$ (**1**) by use of X-ray absorption spectroscopy. This compound is a unique multistable system, which exhibits reversible thermal MMCT phase transition with bistability in the room temperature region [1]. The switching between the low-temperature $\text{Ni}^{\text{III}}-\text{Fe}^{\text{II}}$ phase and the high-temperature $\text{Ni}^{\text{II}}-\text{Fe}^{\text{III}}$ phase is abrupt and characterized by broad hysteresis (280–317 K). XAS spectra were collected for **1** in the temperature range 260–340 K. It allowed us to probe straightforwardly the electronic structures of both metal ions in **1**. When plotting the spectral difference between the high-temperature phase (HT) and low-temperature phase (LT) XAS spectra (Fig. 1), antagonistic features are observed with the complementary roles played by the two metal ions during the charge transfer process.

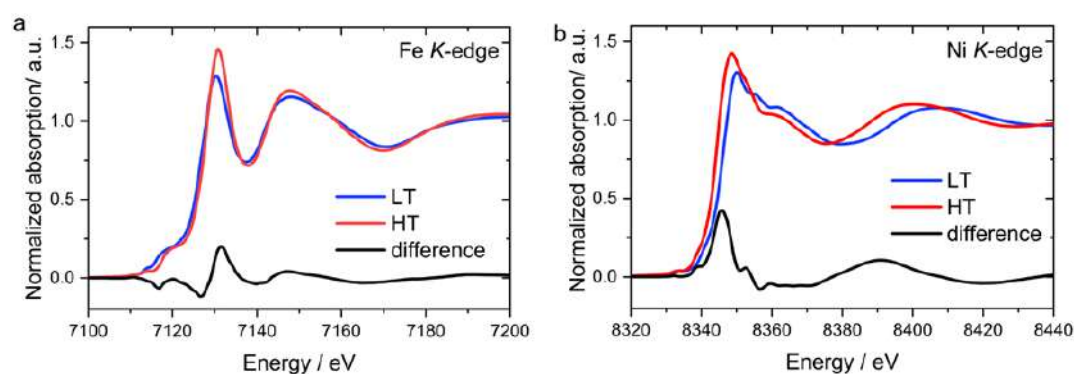


Figure 1: XAS at room temperature (red) and 260 K (blue), and their difference (black) for the Fe (a) and Ni K-edges (b).

[1] M. Reczyński *et al.*, *Angew. Chemie - Int. Ed.*, (2021) 60, 2330

POSTER NO. 34

Improvement of prostate cancer contrast in MRI using core/shell nanoparticles and 9.4T MRI system

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Magnetic Resonance Imaging (MRI) has been used for early cancer detection and treatment monitoring due to its excellent soft tissue contrast. While MRI contrast may be provided solely by tissues themselves, due to differences in their relaxation times, contrast agents shortening T_1 and T_2 relaxation times further improve detection of small pathologies such as early stages prostate cancers.[1, 2] To further improve tumor contrast we have developed new core/shell nanoparticles changing both T_1 and T_2 relaxation times of surrounding water molecules.

The T_1 and T_2 relaxation times of the nanoparticles with various sizes and concentrations were measured at 9.4 T to find the optimum T_1/T_2 ratio for maximum contrast. T_1 - and T_2 -weighted images using core/shell nanoparticles of the animal models prostate cancer were collected. To image mouse with prostate cancer we used 9.4 T MRI system. We imaged 8 weeks nude mice with the tumor before the injection of the targeted and non-targeted contrast agents and in different time after injection (10 min after, 1h, 2h and 24h). The core/shell NPs provided improved tumor contrast when the T_1 and T_2 -weighted MR pulse sequences were applied. The results show that the developed NPs may improve the efficacy of MRI in prostate cancer detection.

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POSTER NO. 35

Star-like hinged grilles: self-similarity and elastic properties

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Gratings (grilles) of rigid hinged bars, constructed in analogy to star patterns in ferroelastics [1], show several levels of self-similarity, i.e. scaling invariance. We found exact formulae for the scaling factors as functions of the shape and of the arms number N of any such star. A minimal set of force constants ensures mechanical stability of the stars with $N = 2$ and $N = 3$. With $N = 4$ the minimal model produces exactly one doubly degenerate mode of vanishing frequency. The reaction of such a star to an external stress applied at a one selected level entails an interesting set of mechanical responses, some of them showing so called negative characteristics, e.g. negative Poisson's ratio or contraction provoked by a tensile load [2]. A human-scale model allowing the reader to palpate the described shape variations will accompany our presentation.

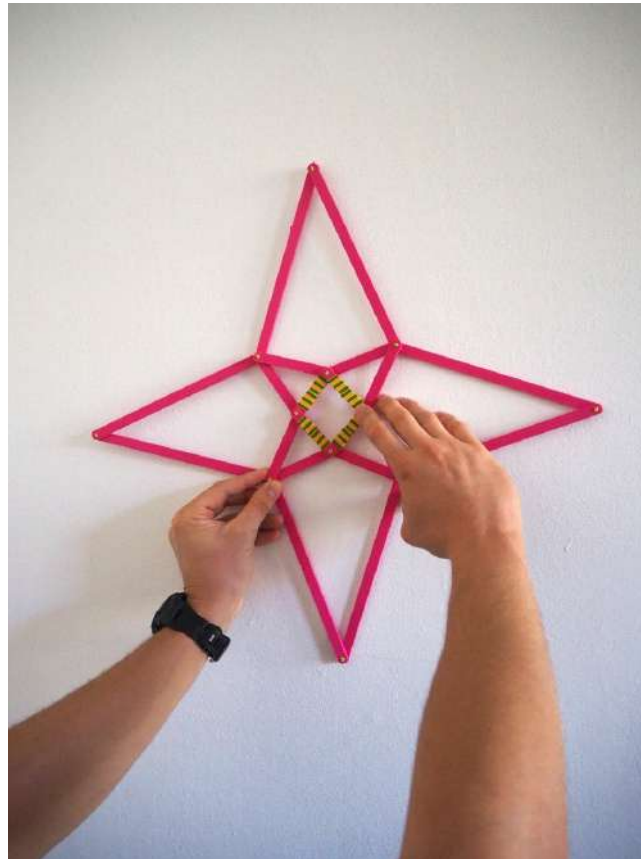


Figure 1: Figure 1. A prototype of human-scale model of a 4 arm star grille [2].

- [1] B. Burzyńska, Physicochemical and structural analysis of organic-inorganic hybrids based on acetamidinium cation, Master Thesis (in Polish), Faculty of Chemistry, University of Wrocław (2023) and references given therein
- [2] P. Sobieszczyk *et al.*, (2024) submitted to *physica status solidi b*