Zakopane School of Physics 2025

Breaking Frontiers: Submicron Structures in Physics and Biology

May 20 – 24, 2025

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Opening lecture, Tue./19:00

Advances in cell migration studies

Z. Rajfur[1], T. Kołodziej[1], O. Adamczyk[1], A. Mielnicka[1,2], and A. Wojciechowski[1]

[1]*Faculty of Physics, Astronomy and Applied Computer Science, Jagiellonian University, ul. prof. Stanisława Łojasiewicza 11, 30-348 Kraków, Poland*
[2]*BRAINCITY, Laboratory of Neurobiology, The Nencki Institute of Experimental Biology PAS, Warsaw, Poland*

email: `zenon.rajfur@uj.edu.pl`

Cell migration (cell motility) is one of the fundamental biological phenomena. It is involved in several biological processes such as wound healing, embryo development, tissue engineering or functioning of immune system. However, many pathological conditions are also connected with disorders in cell migration molecular regulation. The examples of such processes include arthritis, osteoporosis or cancer metastasis. This shows how the knowledge of molecular mechanisms, regulating cell migration, can contribute to invention of novel therapies designed to prevent or cure above mentioned diseases. One of the main experimental tools employed in studies of cell migration is optical microscopy. It is a very versatile experimental tool which allow studies of live cells behavior in their physiological conditions. Recent progress in the development of novel, advanced methods of optical microscopy greatly extends the applicability of this technique in studies of cell migration. One such technique is confocal microscopy which allows to visualize the cell structure and composition in 3D and have a look inside the cell leading to discovery of novel cellular structures [1]. Photoactivation of caged compounds allows to modulate the internal cellular processes in living cells. Analysis of large image data sets elucidates the complex regulation of cellular morphology [2]. Combining optical microscopy with other experimental techniques such as Optically Detected Magnetic Resonance and Traction Force Microscopy gives the prospect of truly multiparametric investigation of cellular functions in live cells [3]. Those developments demonstrate that optical microscopy in connection with other experimental techniques can deliver novel, important information about biological systems.

[1] O. Adamczyk *et al.*, Int. J. Mol. Sci., 22 (2021), 960
[2] A. Mielnicka *et al.*, Sci. Rep. 13 (2023), 15743
[3] T. Kołodziej *et al.*, Biomed. Opt. Express 15 (2024), 4024-4043

SESSION I

Chair: Wojciech Błachucki

09:00	**Yves Kayser** (Mülheim an der Ruhr, Germany) Laboratory-based high energy resolution X-ray spectroscopy	p. 10
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INVITED TALK, WED./09:00

Laboratory-based high energy resolution X-ray spectroscopy

Y. Kayser

Max Planck Institute for Chemical Energy Conversion, Stiftstr. 36-38, 45470 Mülheim an der Ruhr, Germany

email: `yves.kayser@cec.mpg.de`

X-ray absorption spectroscopy (XAS) and X-ray emission spectroscopy (XES) allow probing the electronic and geometric structure of matter. XAS and XES do not only deliver complementary information by probing the unoccupied, respectively the occupied electronic density of states, but depending on the spectral region that is being explored also on the binding distances and partners. The combined information from both analytical techniques can therefore allow a more robust interpretation of the data by disentangling the influence of different parameters on the spectral shape.

The realization of novel X-ray sources and the development of more efficient detection schemes allow the realization of laboratory-based XAS or XES instrumentation [1, 2]. Faster response time, routine characterization measurements, long-term studies and handling of delicate samples are facilitated. Educational and training purposes are other important advantages, as well as the estimation of the achievable sensitivity and discrimination capabilities for measurements realized at large scale facilities, thus increasing the success rate of the experiments performed. The achievable time resolution for dynamical experiments depends on the X-ray source used. With non-pulsed sources, time scales of minutes to hours are accessible, allowing the study of X-ray damage mechanisms, long-term stability, and deactivation processes. Pulsed X-ray sources allow access to dynamics on much shorter time scales and are essentially limited by the pulse duration of the source [3].

[1] W. M. Holden *et al.*, Rev. Sci. Instrum., 88 (2017), 073904
[2] C. Schlesiger *et al.*, J. Anal. At. Spectrom., 30 (2015), 1080
[3] H. Stiel *et al.*, Int. J. Mol. Sci., 22 (2021), 13463

Invited talk, Wed./09:30

Is there really anything new in materials analysis? Spoiler: yes, there is.

Z. Németh, É. Bajnóczi, J. el Guitteoui, A. Mikeházi, and G. Vankó

Wigner Research Centre for Physics, 1525 Budapest, P.O.B. 49., Hungary

email: `nemeth.z@wigner.hu`

Laboratory X-ray source based high-energy-resolution spectrometers have been showing a renaissance that culminated in radical progression recently. Although techniques like X-ray Absorption Near Edge Structure (XANES), Extended X-ray Absorption Fine Structure (EXAFS) or X-ray Emission Spectroscopy (XES) were pioneered mainly on laboratory scale instruments, they have matured dramatically with the advent of synchrotron X-ray sources. The obvious excellence of these large scale photon sources in terms of X-ray brilliance, energy tunability, polarization, pulsed time structure, etc. over the conventional X-ray tubes turned the techniques mentioned dependent almost exclusively on occasionally accessible synchrotron beamtimes. However, the emergence of modern laboratory X-ray tube based spectrometers in the recent decade is being widely recognised, which give rise to a clear demand for such instruments.

Here, an overview will be given on the present status of lab-based high-energy-resolution X-ray spectrometers with selected use cases. Also, an outlook on how this development can be integrated into the anticipated frameworks of innovation?

[1] Z. Németh *et al.*, Rev. Sci. Instrum., 87 (2016), 103105
[2] É.G. Bajnóczi *et al.*, Inorg. Chem., 56 (2017), 14220
[3] Z. Németh *et al.*, Phys. Chem. Chem. Phys., 21 (2019), 9239
[4] Z. Németh *et al.*, J. Synch. Rad., 29 (2022), 1216

CONTRIBUTED TALK, WED./10:00

Multimodal laboratory X-ray spectroscopy setup for material characterization

A. Yakovliev, W. Błachucki, and J. Czapla-Masztafiak

Institute of Nuclear Physics, Polish Academy of Sciences, 152 Radzikowskiego Street, 31-342 Kraków, Poland

email: `artem.yakovliev@ifj.edu.pl`

X-ray spectroscopy probes atomic electronic transition, which are highly specific to chemical composition of the sample and its environment. X-ray fluorescence (XRF) spectroscopy is a low energy resolution technique, which allows to analyze and map chemical composition of the sample with high sensitivity and spatial resolution. On the other hand, high energy resolution techniques, like X-ray absorption (XAS) and X-ray emission (XES) spectroscopy, give insight into the local chemical and structural surrounding of the specific atom of interest. The main drawback of the XAS and XES techniques is that they often require high brilliance sources (i.e. synchrotron facilities and X-ray free electron lasers) in order to obtain good quality spectra. However, in recent years advances in X-ray sources and detectors enabled development of the compact laboratory X-ray spectrometers, providing researchers with an unrestricted access to the XAS/XES experiments [1].

Herein, we report on the development of multimodal XAS/XES/XRF laboratory setup. Double von Hamos geometry-based spectrometer design enables simultaneous XAS and XES data acquisition [2]. Additionally, the combination of silicon drift detector and 3-axis positioning stage allows for XRF based elemental analysis and mapping of the specimen. Altogether, the developed multimodal laboratory X-ray spectroscopy setup is a versatile tool for comprehensive chemical and structural analysis of the wide variety of samples. Examples of spectroscopic studies of small molecule drugs, nanomaterials, and biological tissues will be presented.

[1] P. Zimmermann *et al.*, Coord. Chem. Rev., 423 (2020), 213466
[2] W. Błachucki *et al.*, J. Anal. At. Spectrom., 34 (2019), 1409-1415

Contributed talk, Wed./10:15

Modification of material surface with EUV-induced cold nitrogen plasma

A. Lech, A. Bartnik, P. Wachulak, H. Fiedorowicz, E. Trafny, R. Lewandowski, and A. Wielechowska

Institute of Optoelectronics, Military University of Technology, 2 Kaliskiego St., 00-908 Warsaw, Poland

email: `adam.lech@wat.edu.pl`

The subject of the speech will be the presentation of a unique technique for modifying the surface of material, currently used as a material in implants, with EUV radiation-induced cold plasma. Main goal for using this technique is to receive surfaces with low susceptibility to bacterial adhesion. Obtaining such surfaces is currently considered one of the solutions to the problem of the increased biofilm formation on the surface of surgically located implants.

Surface modification is carried out using a unique laser-plasma EUV source, located at the Laser Technology Department of the Institute of Optoelectronics of the Military University of Technology. EUV plasma-laser source is generated by focusing a Nd:YAG laser beam with a wavelength of 1064 nm, duration of 3 ns and maximum energy of 0.8 J into a double-stream Xe/He gas puff target. The target is formed by pulsed injection of working gas (Xe) and confining gas (He) into the laser focal spot region through two concentric nozzles of the electromagnetic valve system. Then, the produced EUV photons are focused on a sample with the use of an ellipsoidal mirror either directly on the surface of the sample or on a gas portion injected near the sample surface. In the second case, an interaction of the EUV photons with the gas leads to the generation of a photoionized plasma, with relatively low electron temperature. The cold plasma generated in this way is an additional factor, besides EUV radiation, that influences the process of sample surface modification.

To test the effectiveness of EUV-induced cold plasma modification technique three materials were used. The surface of polyetheretherketone (PEEK), Titanium grade 1 and Alumina were measured. Different variants of cold nitrogen plasma modification considered the interaction time of EUV radiation with nitrogen introduced into the system. To verify the effectiveness of the modification technique, after 15 minutes the number of adhered *Staphylococcus aureus* (SA) cells with a concentration of 10^6 CFU/ml was measured. The obtained results show that modification with cold nitrogen plasma induced by EUV pulses could achieve surfaces with a much lower number of adhered bacteria cells, which prevents the formation of bacterial biofilm.

Acknowledgements: Work financed by the project UGB/22-769/2024 WAT "Modyfikacja warstwy wierzchniej biomateriałów z zastosowaniem laserowo plazmowego źródła skrajnego nadfioletu w celu uzyskania powierzchni o niskiej podatności na adhezję mikrobiologiczną"

SESSION II

Chair: Michał Nowakowski

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INVITED TALK, WED./11:30

Protein crystals as nanovehicles for imaging guided phototherapeutics

T.Y. Ohulchanskyy

College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen 518060, Guangdong, China

email: `tyo@szu.edu.cn`

Nanotheranostics is rapidly emerging these days, arising from a combination of diagnostic and therapeutic modalities at the same nanoplatform. In turn, photonanotheranostics may involve optical imaging along with light induced treatment (e.g., photodynamic and photothermal therapies, PDT and PTT). While combination of PDT/PTT can enhance a nanomedicine efficacy [1], nanotheranostics combining PDT / PTT with other therapeutic modalities and optical/multimodal imaging can allow for synergistically enhanced theranostics of cancer with minimal adverse effects [2]. On the other hand, protein crystals, which possess an ordered hierarchical nanostructure, can be introduced as novel delivery vehicles for different drugs, including biopharmaceutical and phototherapeutic ones [3].

This talk will present our results on the development of protein crystals as nanoplatform for theenhanced phototheranostics of cancer. The synthesized protein nanocrystals are loaded with contrast agents for optical/multimodal imaging and therapeutic agents. A synergistic combination of photodynamic and/or photothermal therapies with chemo- and chemodynamic treatments, resulting in an efficient imaging and enhanced therapy of cancer cells in vitro and in animal models in vivo. The talk will conclude with a discussion on the promise of protein nanocrystals for optical bioimaging and nanomedicine.

[1] M. Overchuk *et al.*, ACS Nano, 17 (2023), 7979-8003
[2] A. Grebinyk *et al.*, J. Photochem. Photobiol. C., 58 (2024), 100652
[3] R. Zhou *et al.*, Adv. Drug Deliv. Rev., 216 (2025), 115480

INVITED TALK, WED./12:00

Development of thermoresponsive polymeric nanoparticles loaded with fluorescent and therapeutic agents for enhanced optical bioimaging and cancer therapy

L.O. Vretik[1], A. Yakovliev[2], and T.Yu. Ohulchanskyy[3]

[1] *Taras Shevchenko National University of Kyiv, 01601 Kyiv, Ukraine*
[2] *Institute of Nuclear Physics, Polish Academy of Sciences, 31-342 Kraków, Poland*
[3] *College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen 518060, Guangdong, China*

email: `vretik_l@knu.ua`

Polymeric nanoparticles (PNPs) are among the most frequently used nanocarriers for imaging and therapeutic agents in cancer nanotheranostics [1]. For several years, we have been developing thermoresponsive shell PNPs (TSPNPs) with polysterene core and poly(N-isopropylacrylamide)-based shell that undergoes a reversible conformational transition at 32-40°C (lower critical solution temperature, LCST), leading to a reversible shrinkage of TSPNPs above LCST. When loaded with anticancer molecular drugs and fluorescent dyes, TSPNPs can be used for fluorescence imaging guided cancer therapy [2]. Moreover, shrinkage of TSPNPs at temperatures above LCST and the corresponding aggregation of the nanoparticles affect photophysical properties of fluorescent molecules loaded to TSPNPs (Figure 1), which allows for enhanced fluorescence imaging and photodynamic therapy of cancer [3].

This talk will present the development of TSPNPs, their applications and perspectives for their use in cancer theranostics.

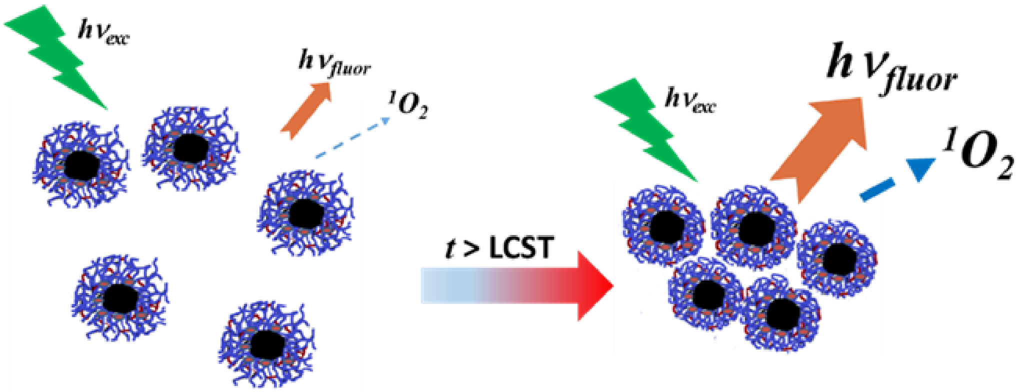

Figure 1: Scheme illustrating an effect of temperature rise on fluorophores in TSPNPs [3].

[1] S.M. Hosseini *et al.*, Mater. Today Chem., 29 (2023), 101400
[2] O.M. Chepurna *et al.*, J. Nanobiotechnology, 18 (2020), 19
[3] O. Chepurna *et al.*, Nanoscale Adv., 7 (2025), 1946

Contributed talk, Wed./12:30

Cu@O composite particles decorated with Ag nanoparticles - formation mechanism and antimicrobial properties

O. Polit, Ż. Świątkowska-Warkocka, and M. S. Shakeri

Institute of Nuclear Physics Polish Academy of Sciences, PL-31342 Kraków, Poland

email: `oliwia.polit@ifj.edu.pl`

Cu@O submicrometer composite particles doped with 5% Ag synthesized by pulsed laser irradiation in liquid method (PLIL). PLIL is a clean, one-step method that enables control of particle size, composition and morphology without the use of chemical reducing agents that can be difficult to remove and potentially toxic to tissues and the environment. The resulting composites were comprehensively characterized with techniques such as transmission electron microscopy (TEM), X-ray diffraction (XRD), X-ray absorption spectroscopy (XAS) and others, to evaluate their structural, morphological, and optical properties. The addition of Ag nanoparticles enhanced the antimicrobial efficacy and optical properties of the Cu-based composite particles. These composites demonstrated potent antibacterial and antifungal activity against representative pathogens, highlighting their potential for addressing antibiotic-resistant infections and potential for other applications.

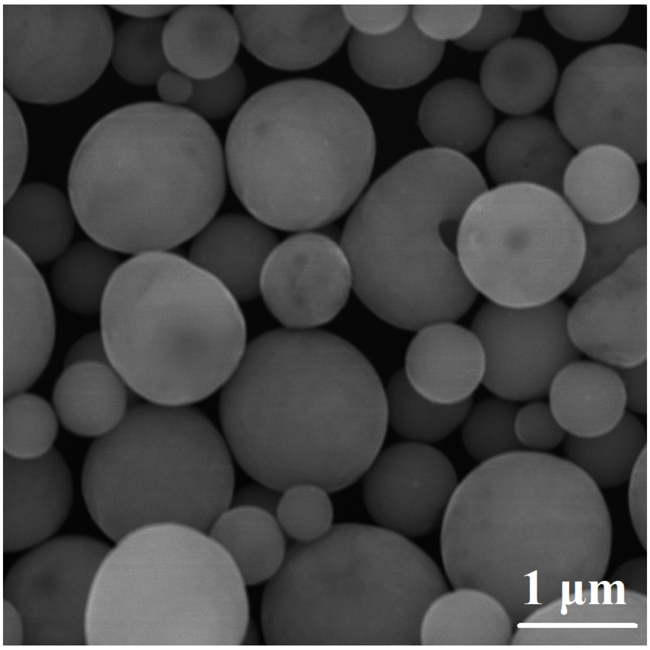

Figure 1: Example of scanning electron microscope image for one sample of the synthesized Cu-O-Ag particles.

Contributed talk, Wed./12:45

Thermal characterisation, dielectric relaxation and X-ray diffraction studies of selexipag

S. Sureshkumar, A. Deptuch, A. Drzewicz, and P.M. Zieliński

Department of Soft Matter Research, Institute of Nuclear Physics Polish Academy of Sciences, Radzikowskiego 152, 31-342 Kraków, Poland

email: `sumesh.sureshkumar@ifj.edu.pl`

Selexipag (SLP) is an active pharmaceutical ingredient used for the treatment of pulmonary arterial hypertension. The present work examines the thermal characteristics of selexipag (SLP) in both crystalline and amorphous forms using thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). Key thermodynamic parameters, including Vogel temperature (T_0), glass transition temperature (T_g), strength parameter (D), kinetic fragility index (m), and apparent activation energy (E_a), were derived using a variety of theoretical isoconversional methods of kinetic analysis, including those by Kissinger-Akahira-Sunose (KAS), Flynn-Wall-Ozawa (FWO), and Moynihan (MYN). The relaxation processes were examined in greater detail using broadband dielectric spectroscopy (BDS). We identified three different relaxations: structural relaxation α and secondary relaxations β and γ processes. The non-Debye relaxation behaviour of the SLP is described using the Havriliak-Negami model. The stretching parameter (β_{KWW}) from the Kohlrausch-Williams-Watts (KWW) formalism is used as a probe to examine the heterogeneity of molecular mobility near the transition temperature. All of the aforementioned thermodynamic parameters, as well as the activation energy related to secondary processes, have been effectively determined by using the Vogel-Fulcher-Tammann (VFT) and Arrhenius equations. We employed X-ray diffraction to look into the recrystallisation tendencies of SLP. The amorphous SLP showed no evidence of crystallisation and was stable in XRD. The results could provide important information about stability and insights for improving the formulation and shelf life of amorphous selexipag.

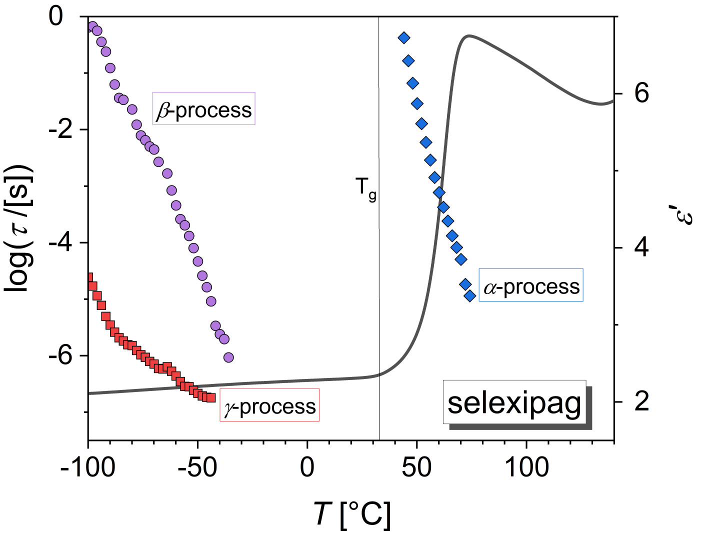

Figure 1: Temperature dependence of the real part of the complex dielectric function and the logarithm of the characteristic relaxation time

[1] A. Dołęga and P. M. Zieliński, J. Non-Cryst. Solids, 575 (2022), 121198
[2] S.P. Bhardwaj *et al.*, Mol. Pharm., 10 (2013), 694-700

SESSION III

Chair: Petr Neugebauer

14:00	**Aldona Mzyk** (Kongens Lyngby, Denmark) Nanodiamond-based quantum sensing in biomedical applications	p. 20
14:30	**Yann Garcia** (Louvain-la-Neuve, Belgium) Coordination complexes as electronic detectors	p. 21
15:00	**Naveen Kumar Chogondahalli Muniraju** (Kraków, Poland) Integrating molecular magnets into polymers: electrospun composites with tunable charge-transfer transitions	p. 22
15:15	**Aleksandra Pacanowska** (Kraków, Poland) Pressure-induced metal-to-metal electron transfer in molecular chain composite material probed by X-ray absorption spectroscopy	p. 23
15:30	**Ali Darwich** (Košice, Slovakia) Incommensurate modulated crystal structure as a source of two-dimensional magnetic disorder in the quantum magnet $Cu(tn)Cl_2$	p. 24

Invited talk, Wed./14:00

Nanodiamond-based quantum sensing in biomedical applications

A. Mzyk

Technical University of Denmark, Kgs. Lyngby, Ørsteds Plads, 2800, Denmark

email: `ailmz@dtu.dk`

Sparkling, hard and durable, these are some of the properties commonly associated with diamonds. These qualities have made them desirable within our society for centuries. In research, the unique properties of diamonds have drawn in many enthusiasts. Particularly, nanodiamonds with crystal lattice defects such as the negatively charged nitrogen-vacancy (NV-) centers, which have emerged as powerful and versatile quantum sensors [1]. This talk focuses on a specific way to use the quantum-based sensing properties of nanodiamond with ensembles of NV- centers, a technique called relaxometry (or T1) and its application in cell biology to detect free radicals (FRs) [2]. FRs are omnipresent and one of the key players in cellular signalling. Despite their relevance, information about FRs is sparse and therefore their use as clinical biomarkers is severely limited. Since FRs are short lived and reactive, it is challenging to detect them with the state-of-the-art methodology. In my talk I will address a few exciting examples of biological processes and their clinical relevance where the role of free radicals was explored with T1 relaxometry. I will stimulate discourse on the future of nanodiamond-based quantum sensing and how it can open new perspectives in cell biology, drug screening and clinical diagnostics.

[1] A. Mzyk *et al.*, Anal. Chem., 94 (2021), 225-249
[2] A. Mzyk *et al.*, Acc. Chem. Res., 55 (2022), 3572-3580

Invited talk, Wed./14:30

Coordination complexes as electronic detectors

Y. Garcia

Institute of Condensed Matter and Nanosciences (IMCN/MOST), Place Louis Pasteur 1,
1348 Louvain-la-Neuve, Belgium

email: `yann.garcia@uclouvain.be`

In recent years, much attention has been focused on the efficient detection of chemical pollutants, especially volatile organic compounds (VOCs) and hazardous gases (HGs), using various e-sensors. Such toxic molecules emitted in urban environments are threatening the quality of our daily life. In particular, the detection of relatively small volatile molecules at room temperature, is difficult at low concentration levels, and therefore highly sensitive sensors, preferably produced at low cost, are needed.

Our laboratory has recently developed a series of iron coordination complexes that were tested as detectors of toxic industrial chemicals. For example, the mononuclear complex $[Fe(Hbta)_2(H_2O)_2]\cdot 2H_2O$ (1) (Hbta = bis(1H-tetrazol-5-yl)amine), was shown to be able to detect in less than 10 min, with a high selectivity and ultra-sensitivity, 32 different VOCs and HGs [1]. The detection is accompanied by significant and fast colour changes detectable by simple standard chemometric means using a handful smartphone-based analytical method. The crystal lattice of this material reconstructs after adsorbing VOCs vapours, reconstruction which is accompanied by a spin state and a colour change, which was tracked by several physical methods. In addition to its high thermal stability (up to 175 °C), the colorimetric sensor showed excellent reusability by consecutive cycles of adsorption-desorption. This sensor is low-cost, environmentally friendly, easy to use, and shows excellent and fast detection performances. Such features offer attractive prospects to use this material and others [2, 3], for in-field detection and food safety control in environmental conditions.

[1] L. Sun *et al.*, J. Hazardous Mater., 437 (2022), 129364

[2] L. Sun *et al.*, In 'Mössbauer Spectroscopy: Applications in Chemistry and Materials Science', Wiley VCH 2024

[3] W. Li *et al.*, J. Mater. Chem. C, 11 (2023), 11175

Contributed talk, Wed./15:00

Integrating molecular magnets into polymers: electrospun composites with tunable charge-transfer transitions

A. Pacanowska[1], W. Sas[1], Ł. Gondek[2], M. Fitta[1], and C.M.N. Kumar[1]

[1]*Institute of Nuclear Physics Polish Academy of Sciences, Radzikowskiego 152, 31-342 Kraków, Poland*
[2]*AGH University of Krakow, Faculty of Physics and Applied Computer Science, 30-059 Kraków, Poland*

email: `naveen.chogondahalli@ifj.edu.pl`

We present the synthesis and characterization of composite fibers incorporating RbxMn[Fe(CN)$_6$]_(2+x)/3·nH$_2$O Prussian blue analogue (PBA) microcrystals into a polyvinylpyrrolidone (PVP) matrix via electrospinning. Three compositions with varying rubidium content (x $\approx$ 0.94, 0.77, 0.49) were prepared and structurally confirmed to retain the high-temperature cubic framework after polymer embedding, as demonstrated by powder X-ray diffraction and Rietveld refinement. Scanning electron microscopy confirmed uniform incorporation of microcrystals within the fibers, and energy-dispersive X-ray spectroscopy verified their stoichiometry. X-ray absorption spectroscopy at the Fe and Mn K-edges showed that polymer integration did not significantly affect the local electronic structure. Magnetization measurements revealed that the composites preserved the characteristic thermal charge-transfer transition (Fe^{3+}-Mn^{2+} $\leftrightarrow$ Fe^{2+}-Mn^{3+}) near room temperature. Importantly, the thermal hysteresis associated with this transition was significantly broadened in the composites, indicating strong elastic coupling between the microcrystals and the polymer host.

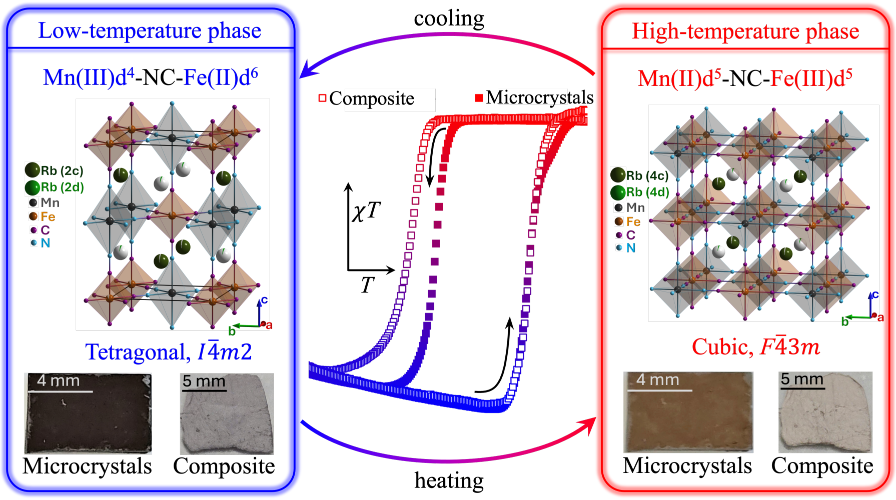

Figure 1: The temperature-induced transition in an Rb-based Prussian blue analogue that simultaneously manifests both electronic and structural bistabilities. This transition, driven by a reversible Fe/Mn intervalence charge transfer, switches the system from a cubic phase to a tetragonal phase. Magnetization thermal hysteresis is enhanced in the composite.

Contributed talk, Wed./15:15

Pressure-induced metal-to-metal electron transfer in molecular chain composite material probed by X-ray absorption spectroscopy

A. Pacanowska[1], G. Wota[2], N. K. Chogondahalli Muniraju[1], A. Maximienko[3], W. Tabiś[4], B. Nowicka[2], and M. Fitta[1]

[1] *Institute of Nuclear Physics PAS, Radzikowskiego 152, 31-342 Kraków, Poland*
[2] *Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Kraków, Poland*
[3] *SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, Czerwone Maki 98, 30-392 Kraków, Poland*
[4] *Faculty of Physics and Applied Computer Sciences, AGH University of Kraków, al. Mickiewicza 30, 30-059 Kraków, Poland*

email: `aleksandra.pacanowska@ifj.edu.pl`

The following study investigates the pressure-induced metal-to-metal charge transfer (MMCT) transition in $\{NH_4[Ni(cyclam)][Fe(CN)_6]\cdot 5H_2O\}_n$ coordination chain [1] microcrystals embedded in polycaprolactone foil (NiFe-foil), prepared via drop-casting, aimed at pressure sensor applications. The research examines the transition within two stable phases under applied external pressure at room temperature (Figure 1A). X-ray absorption spectroscopy at the Fe and Ni K-edges, provided detailed insights into the pressure-induced oxidation state changes in metal centers at RT of NiFe-foil (Figure 1B), validated by additional XAS measurements at low (250 K) and high (312 K) temperatures, using custom-made sample holder. These findings underscore the promising potential of NiFe-foil composites as advanced materials for pressure sensors, showcasing their response to external stimuli and their ability to undergo reversible phase transition.

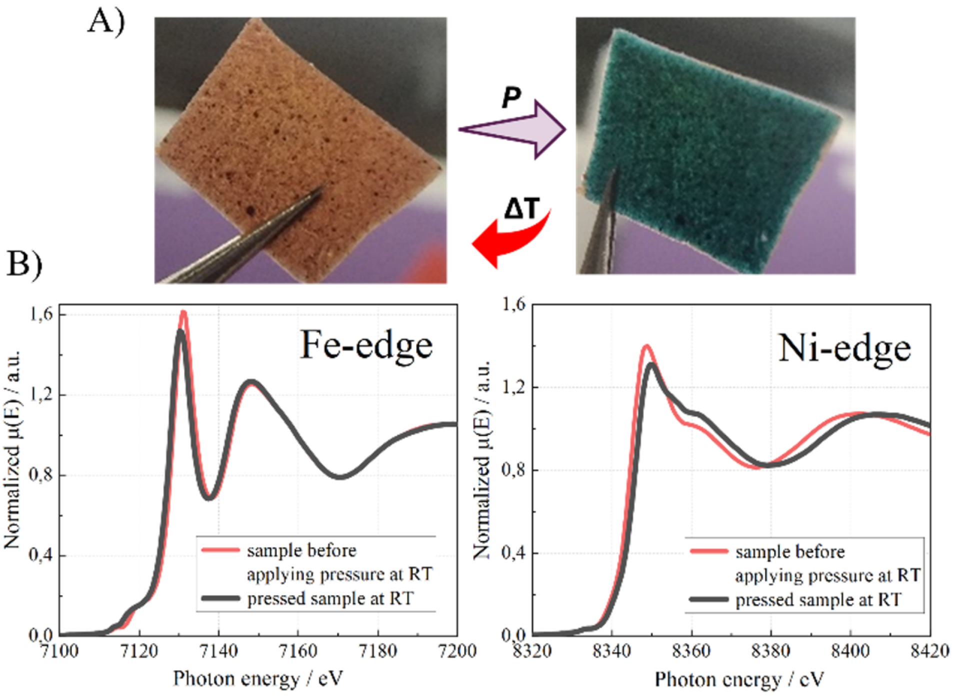

Figure 1: A) Photographic representation of NiFe-foil before (brown) and after (dark blue) applying external pressure. B) Antagonistic changes of normalized μ(E) at Fe (left) and Ni (right) K-edges due to the pressure-induced MMCT for NiFe-foil.

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

Contributed talk, Wed./15:30

Incommensurate modulated crystal structure as a source of two-dimensional magnetic disorder in the quantum magnet $Cu(tn)Cl_2$

A. Darwich, R. Tarasenko, M. Orendáč, and A. Orendáčová

Institute of Physics, P. J. Šafárik University, Park Angelinum 9, 04001 Košice, Slovakia

email: `email`

Previous experimental studies of $Cu(tn)Cl_2$ ($tn = C_3H_{10}N_2$) revealed a structural phase transition to an incommensurate modulated structure [1]. Decreasing the temperature down to 120 K, the structure goes from a disorder over two *tn* positions to a locked stable modulation with two conformations. The low temperature structure can be approximated as a set of “four domains” which have two orientations of *tn* ligands and thickness of 1, 4, 4, 1 unit cells, periodically propagating along *b* axis. Considering the crucial role of *tn* positions in the formation of exchange pathways as revealed previously by first principle studies, different exchange couplings can be expected within these two-dimensional domains. Which may be responsible for the prevalence of two-dimensional magnetic behavior observed by specific heat studies and muon spin relaxation down to 40 mK. Considering two strongest nearest neighbor exchange couplings provided by first principle calculations forms effective rectangular lattice. While excellent agreement between specific heat data and the theory was achieved, significant deviations appear in the description of magnetic susceptibility and magnetic phase diagram. Negligible broad hump at about 0.55 K in specific heat data is an indicator of some phase transition. No traces of hysteresis below this temperature exclude a possibility of the onset of spin glass phase.

Acknowledgements: Financial support of projects VEGA 1/0132/22, APVV-18-0197 and APVV-22-0172 is acknowledged.

[1] C.A. Corrêa *et al.*, J. Phys. Chem. C, 126 (2022), 14573-14580

SESSION IV

Chair: Yann Garcia

16:30	**Petr Neugebauer** (Brno, Czech Republic) Introduction to magnetic resonance, applications and future	p. 26
17:00	**Kamil Stachurski** (Kraków, Poland) Characterization of ischemic stroke using magnetic resonance imaging for theranostic applications	p. 27
17:15	**Marianna Makova** (Bratislava, Slovak Republic) Brain changes induced by maternal depression: a magnetic resonance study	p. 28

Invited talk, Wed./16:30

Introduction to magnetic resonance, applications and future

P. Neugebauer, O. Laguta, V. Santana, J. Dubský, J. Navarro, L. Kotásková, A. Sojka, M. Šedivý, J. Hrubý, A. Fanisaberi, L. M. Tahsin, Š. Fuks, Š. Zelníček, and P. Pelikán

CEITEC — Central European Institute of Technology, Vysoké učení technické v Brně, Purkyňova 123, 61200 Brno, Czech Republic

email: `neugebauer@vutbr.cz`

Magnetic resonance is a widespread method in various, not only scientific, branches. It is a method generally known to most of society from the non-hospital environment; mainly, images of the brain taken by the magnetic resonance imaging (MRI) method have been seen by almost everyone. Its broad capabilities and possibilities are perhaps best evidenced by the number of Nobel Prizes awarded for its development (6 prizes) and the knowledge that would not have been made without it (4 prizes). During the lecture, the principle of the method will be simply explained on the hydrogen atom (H - composed of one electron orbiting an atomic nucleus formed by a proton), one of the basic stones of life, H_2O (water). The listener will be introduced to nuclear magnetic resonance (NMR), the lesser-known electron spin resonance (ESR) [1]. Furthermore, a method that uses both magnetic resonance techniques NMR and ESR to amplify (improve) the signal using nuclear dynamic polarization (DNP) [2]. The rich history of magnetic resonance in the Czech and former Czechoslovakian Republics, mainly associated with Tesla Brno, and the current global development and future will be mentioned (Figure 1) [3].

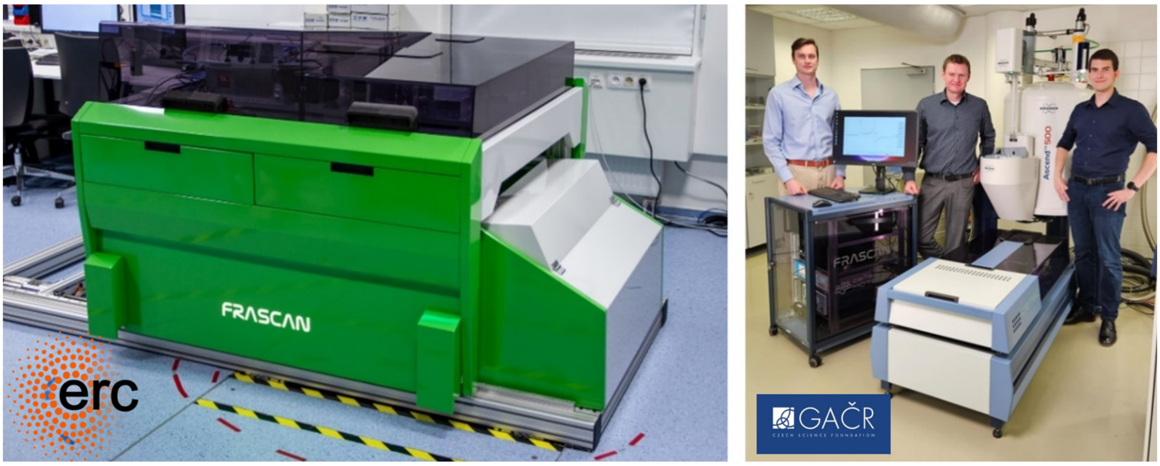

Figure 1: Left: Photo of the first high-frequency ESR spectrometer (FRASCAN) designed and assembled at CEITEC BUT Brno by Petr Neugebauer's team. Left: Implementation of the high-frequency ESR spectrometer into widely used NMR magnets (FRASCAN II), in the photo from left Dr. Oleksii Laguta, doc. Dr. Ing. Petr Neugebauer and Ing. Jan Dubský.

[1] A. Sojka *et al.*, RSC Electron Paramagnetic Resonance, 27 (2020), 214-252
[2] P. Neugebauer *et al.*, Phys. Chem. Chem. Phys., 16 (2014), 18781-18787
[3] J. Dubský *et al.*, Appl. Magn. Reson., 55 (2024), 1047-1064

Contributed talk, Wed./17:00

Characterization of ischemic stroke using magnetic resonance imaging for theranostic applications

K. Stachurski[1], K. Jasiński[1], K. Kalita[1], B. Pomierny[2], P. Rachwał[2], Z. Guzda[3], J. Jurczyk[3], P. Warszyński[4], and W. P. Węglarz[1]

[1] *Institute of Nuclear Physics PAS, Department of MRI, 31-342 Kraków, Poland*
[2] *Jagiellonian University Medical College, Department of Toxicological Biochemistry, 30-688 Kraków, Poland*
[3] *Jagiellonian University Medical College, Department of Toxicology, 30-688 Kraków, Poland*
[4] *Institute of Catalysis and Surface Chemistry PAS, 30-239 Kraków, Poland*

email: `kamil.stachurski@ifj.edu.pl`

Ischemic stroke remains a significant clinical challenge, requiring effective diagnostic and therapeutic methods. The middle cerebral artery occlusion (MCAO) animal model is widely used in preclinical studies to replicate stroke pathophysiology and evaluate potential therapies [1]. This study focuses on the characterization of pathological changes in the MCAO model using advanced magnetic resonance imaging (MRI) techniques in the context of future theranostic applications.

A detailed analysis of MRI parameters was conducted, including diffusion-weighted imaging (DWI), apparent diffusion coefficient (ADC) mapping, blood-brain barrier (BBB) permeability assessment and relaxation mapping (T1 and T2). The obtained results allowed for the determination of the temporal dynamics of ischemic changes, identification of the infarct core and penumbra and monitoring of blood-brain barrier permeability. Additionally, an optimized measurement protocol was developed for the biodistribution studies of a contrast agent in ischemic stroke and the detection limit of the contrast agent within the ischemic region was determined using MRI.

The results indicate significant differences in relaxation and diffusion parameters as well as in the biodistribution of the contrast agent within the ischemic area. The MRI-based temporal characterization enables better therapeutic strategy adjustments and optimization of the biodistribution of future theranostic nanoparticles. The integration of MRI imaging with the evaluation of new theranostics may contribute to the development of novel and effective treatment methods for ischemic stroke.

Acknowledgements: This work was partially supported by the National Centre of Science (NCN) of Poland, under grant nr: 2020/39/NZ7/01913 (OPUS-20).

[1] B. Pomierny *et al.*, Biomed. Pharmacother., 170 (2024), 116102

Contributed talk, Wed./17:15

Brain changes induced by maternal depression: a magnetic resonance study

M. Makova

Institute of Physical Chemistry and Chemical Physics, Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava, Radlinského 9, SK-812 37 Bratislava, Slovak Republic

email: `marianna.makova@stuba.sk`

Maternal depression and its treatment can induce changes in regional brain morphology and neurochemistry. Many of these changes can be transferred to their offspring or induce additional negative changes [1]. The study aims to investigate neurochemical and structural changes induced by chronic stress, as a model of depression, in rat dams and their offsprings. The effect of antidepressant treatment was studied subsequently.

In vivo magnetic resonance (MR) imaging and localized proton MR spectroscopy were performed at 4.7 T. Structural analysis utilized T2-weighted fast spin echo imaging, followed by a semi-automated volumetric analysis using Advanced Normalization Tools and MRtrix3 in C++. The Waxholm Space atlas v4 served as a reference for quantifying brain regions. Metabolic concentrations were quantified from the dorsal hippocampus using ^{1}H MR spectroscopy, with spectra acquired using a SPECIAL localization sequence and automatically quantified in LC model.

In vivo spectroscopy revealed that stress affected the GABAergic system in the hippocampus of rat dams, with potential antidepressant-related improvement. On the other hand, changes in N-acetylaspartate (NAA), a key marker of neuronal integrity and mitochondrial function, were observed in offsprings of antidepressant-treated dams. MR imaging revealed no changes in hippocampal volume in stressed dams; however, larger amygdala volume was found, potentially due to increased neuronal activity or increased synaptic density. Furthermore, maternal stress affected amygdala and hippocampus volumes in offspring.

These findings suggest that maternal depression and even antidepressant treatment during pregnancy may have adverse effects on offspring.

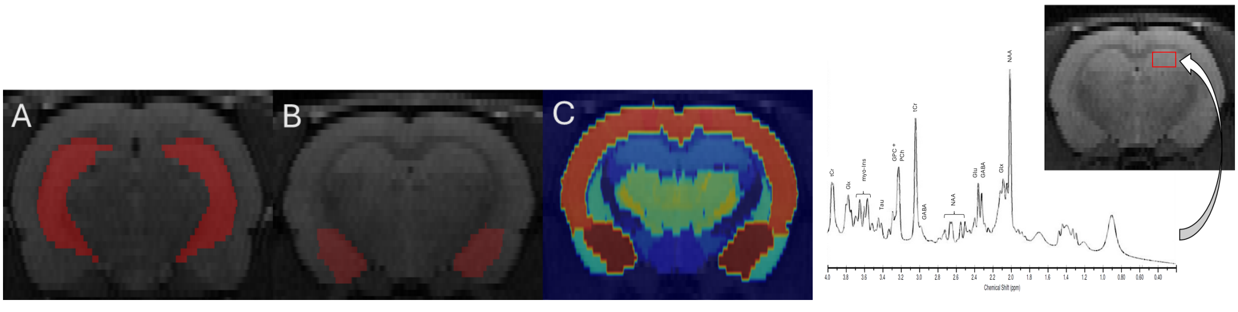

Figure 1: *Left:* MR images of a rat brain with highlighted regions of interest (A) hippocampus; (B) amygdala; (C) whole brain. *Right:* Representative ^{1}H MR spectrum from rat dorsal hippocampus processed with LC Model. γ-aminobutyrate (GABA); choline compounds (GPC+PCh); glutamate (Glu); glutamine (Gln); myo-inositol (myo-Ins); N-acetylaspartate (NAA); taurine (Tau) and total creatine (tCr).

Acknowledgements: The study was supported in part by the VEGA 02/0057/22, APVV-21-0299 and the call for doctoral students and young researchers of Slovak University of Technology in Bratislava to start a research career Grant 23-04-08-A.

[1] P.J. Brunton, Reproduction, 146 (2013), 175-189.

SESSION V

Chair: Wojciech Gawełda

14:30	**Ewelina Lipiec** (Kraków, Poland) Mind the gap! Plasmonic nanocavity for trapping of local molecular rearrangements in selected biomolecules	p. 30
15:00	**Rafał Luchowski** (Lublin, Poland) The macula - the center of precise vision. Why is it crucial for our eye?	p. 31
15:30	**Dawid Lupa** (Kraków, Poland) Quantitative Nanomechanical Mapping reveals nanoscale topographical and mechanical heterogeneity in inner mitochondrial membrane	p. 32
15:45	**Monika Szczpanek-Dulska** (Kraków, Poland) Mechanosensitivity of microglia: impact of substrate stiffness on single cells morphology and migration	p. 33

Invited talk, Thu./14:30

Mind the gap! Plasmonic nanocavity for trapping of local molecular rearrangements in selected biomolecules

E. Lipiec[1], A. Cernescu[2], A. Chahaj-Brekiesz[3], M. Czaja[1,4], D. Ghosh[5], J. Kaderli[5], J. Kobierski[6], D. Lupa[1], D. Perez-Guaita[7], R. Riek[5], S. Seweryn[1,4], K. Skirlińska-Nosek[1,4], K. Sofińska[1], A. Wnętrzak[3], R. Zenobi[8], and M. Szymoński[1]

[1] *Jagiellonian University, Faculty of Physics, Astronomy and Applied Computer Science, M. Smoluchowski Institute of Physics, Łojasiewicza 11, 30-348 Kraków, Poland*
[2] *Attocube Systems AG, Eglfinger Weg 2, 85540 Haar, Germany*
[3] *Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Kraków, Poland*
[4] *Jagiellonian University, Doctoral School of Exact and Natural Sciences, Kraków, Poland*
[5] *Laboratory of Physical Chemistry, ETH Zürich, 8093 Zürich, Switzerland*
[6] *Faculty of Pharmacy, Jagiellonian University Medical College, 31-007 Kraków, Poland*
[7] *Centre for Biospectroscopy and School of Chemistry, Monash University 3800, Victoria, Australia*
[8] *Department of Chemistry and Applied Biosciences, ETH Zürich, 8093 Zürich, Switzerland*

email: `ewelina.lipiec@uj.edu.pl`

Despite several decades of research, the molecules of life: nucleic acids, proteins, and lipids hide many secrets from us. Due to the lack of efficient sensitivity and spatial resolution of conventional analytical techniques, the properties of such molecules, heterogeneous at the nanoscale, are still not fully explored.

Hence, to achieve significant progress in the characterization of the biomolecules, research on processes occurring in plasmonic nano-gap junctions must be performed, providing solid information on the generation of surface plasmons, near-field confinement of the generated electromagnetic field by the nanojunction/cavity, as well as the field enhanced molecule vibronic excitations, Raman scattering, and infrared transitions in the nano-gap junction. All those fundamental subjects are at the base of modern molecular nanospectroscopies: Tip-Enhanced Raman Spectroscopy (TERS) and Fourier Transform InfraRed nano-spectroscopy.

Our findings involve the nanospectroscopic investigation into the local secondary structure of aggregating Alzheimer's proteins and peptides. Several significant aspects will be discussed such as: i) monitoring of the nanoscale distribution of β-sheet secondary structure for revealing the aggregation pathway of amyloid-β [1], ii) an effect of the anti-aggregation drug called bexarotene on protein aggregates [2], iii) pioneering measurements of amyloid-β in liquid and the protective role of solvent [3], iv) local molecular rearrangements upon tau protein fibrillation [4]. Since lipids may affect secondary structure of aggregating amyloids a comparison of AFM-TERS and STM-TERS in nanospectroscopic maping of lipid monolayers for revealing of local molecular distribution, phase separation, and formation of domains will be also presented [5].

Acknowledgements: This work is supported by the National Science Centre, Poland under the OPUS 19 project (Reg No UMO 2020 37 /B/ST 4 02990)

[1] E. Lipiec *et al.*, Angew. Chem. Int. Ed., 130 (2018), 8655-8660
[2] K. Sofińska *et al.*, Nanoscale, 15 (2023), 14606-14614
[3] E. Lipiec *et al.*, Angew. Chem. Int. Ed., 60 (2021), 4545-4550
[4] K. Sofińska *et al.*, Nanoscale, 16 (2024), 5294-5301
[5] K. Sofińska *et al.*, Adv. Colloid Interface Sci., 301 (2022), 102614

INVITED TALK, THU./15:00

The macula - the center of precise vision. Why is it crucial for our eye?

R. Luchowski[1], W.I. Gruszecki[1], W. Grudzinski[1], R. Welc-Stanowska[1], A. Sek[1], M.M. Mendes Pinto[1], J. Ostrowski[2], K. Sowinski[1], and R. Rejdak[2]

[1]*Department of Biophysics, Institute of Physics, Maria Curie-Sklodowska University, pl. M. Curie-Sklodowskiej 1, 20-031 Lublin, Poland*
[2]*Department of General Ophthalmology, Medical University of Lublin, ul. Chmielna 1, Lublin, Poland*

email: `rafal.luchowski@umcs.pl`

The human eye must effectively adapt to varying light conditions, which is quite challenging. It must be sensitive enough for low-light situations yet stable under bright light. To achieve this, the eye employs mechanisms to regulate the amount of light reaching its light-sensitive cells (photoreceptors). The studies conducted in our lab has revealed that two pigments, lutein and zeaxanthin, located in a specific part of the retina known as the macula, operate similarly at the molecular level. We refer to this process as "molecular blinds” [1]. Essentially, these pigments act like a switch, blocking excessive light in bright conditions and allowing more light through when it’s darker. This mechanism works by altering the shape of these pigments upon exposure to light: in bright light, they adopt one shape (*cis*), which blocks some light, and in dimmer conditions, they switch to another shape (*trans*), allowing more light to pass through. In the presentation, it will shown data on how lutein and zeaxanthin are specifically involved in this "molecular blinds" mechanism. Additionally, I’ll illustrate and discuss a diagram where these pigments are situated in the macula and their role in regulating the eye’s light sensitivity.

Acknowledgements: Acknowledgments to Nacional Science Center for grant funding # 2022/45/B/NZ1/00612

[1] R. Luchowski *et al.*, J. Phys. Chem. B, 125 (2021), 6090-6102

CONTRIBUTED TALK, THU./15:30

Quantitative Nanomechanical Mapping reveals nanoscale topographical and mechanical heterogeneity in inner mitochondrial membrane

D. Lupa[1], A. Chachaj-Brekiesz[2], A. Wnętrzak[2], and E. Lipiec[1]

[1] *Jagiellonian University, Faculty of Physics, Astronomy, and Applied Computer Science, M. Smoluchowski Institute of Physics, Łojasiewicza 11, 30-348 Kraków, Poland*
[2] *Jagiellonian University, Faculty of Chemistry, Gronostajowa 2, 30-387 Kraków, Poland*

email: `dawid.lupa@uj.edu.pl`

Lipid membranes are essential structures present in all living cells, regardless of their origin or function. Their primary role is to define cell boundaries and influence the cell's overall mechanical stiffness. In eukaryotic cells, membranes also enclose organelles, enabling compartmentalization that is vital for maintaining cellular homeostasis. At the nanoscale, lateral distribution of lipids within membranes is uneven, leading to the formation of dynamic assemblies known as lipid rafts.

Traditional analytical techniques struggle to resolve the topographical and mechanical characteristics of lipid membranes due to limitations imposed by membrane thickness (approximately 5 nm) and the Abbe diffraction limit. To overcome these challenges, atomic force microscopy (AFM) is commonly applied, offering high-resolution insights into the topography and nanomechanical behavior of supported lipid mono- and bilayers.

In this study, we extend the capabilities of AFM nanoindentation to probe lipid monolayers - models that represent a single membrane leaflet under physiologically relevant conditions. This is done by applying quantitative nanomechanical mapping working in a subnanometer indentation regime. Based on elastic contact theory, we obtain maps of topography, elastic modulus, and adhesion force for both single-component lipid layers and a model of the inner mitochondrial membrane (IMM). A clear correlation between surface topography and mechanical properties is demonstrated. The findings are interpreted in terms of lipid acyl chain conformations and phase separation.

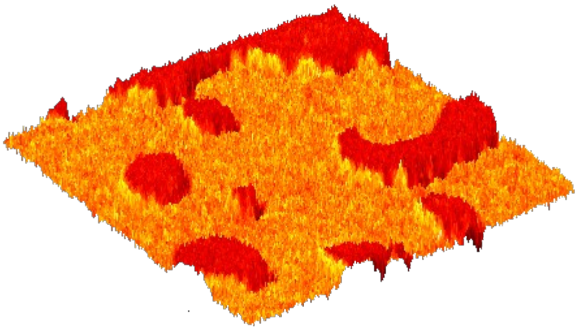

Figure 1: Topographical AFM image of IMM with elastic modulus overlay.

Acknowledgements: This work is supported by the National Science Centre, Poland under the "OPUS 19" project (Reg. No. UMO-2020/37/B/ST4/02990).

CONTRIBUTED TALK, THU./15:45

Mechanosensitivity of microglia: impact of substrate stiffness on single cells morphology and migration

M. Szczepanek-Dulska[1], K. Berghauzen-Maciejewska[1], K. Dulski[2], and K. Pogoda[1]

[1]*Institute of Nuclear Physics Polish Academy of Sciences, Radzikowskiego 152, 31-342 Kraków, Poland*
[2]*Faculty of Physics, Astronomy and Applied Science, Jagiellonian University, Łojasiewicza 11, 30-348 Kraków, Poland*

email: `monika.szczepanek@ifj.edu.pl`

The brain, as one of the softest tissues in the body, exhibits heterogeneous mechanical properties that change with aging and pathology development [1]. Microglia, the most abundant immune cells in the brain, play a crucial role in neural tissue remodeling under both physiological and pathological conditions [2]. To investigate their mechanoresponsiveness, we cultured microglial cells on polyacrylamide (PAA) substrates with varying stiffnesses that mimic brain's mechanical environment.

Our study focused on the influence of substrate stiffness on cell morphology and migration. We classified distinct cell shapes, migration modes, and the ratio of static to dynamic cells as a function of substrate mechanical properties. Dynamic cells were further categorized based on their traveled distance, and a modified persistent random walk (PRW) model [3] was applied to determine their persistence time. Our results indicate that amoeboid morphology, a potential marker of microglial activation, is mostly prominent at 5 kPa substrate stiffness, where the highest persistence time was observed. Softer substrates led to actin cytoskeleton disorganization, while stiffer substrates promoted actin polymerization, consistent with previous findings in other cell types. Microglia cultured on high substrate stiffnesses displayed increased migration speed, persistence time, and end-to-end displacement compared to those on softer ones.

Moreover, we observed a shift in population heterogeneity with increasing substrate stiffness — cells appeared more homogeneous on soft substrates, but exhibited greater phenotypic diversity as stiffness increased. These findings suggest that mechanical cues modulate microglial behavior in a stiffness-dependent manner, which may have implications for understanding their role in aging and disease.

[1] I. Levental *et al.*, Soft Matter, 3 (2007), 299
[2] C. Gao *et al.*, Sig. Transduct. Target. Ther., 8 (2023), 359
[3] P. Maiuri *et al.*, Cell, 161 (2015), 374-386

SESSION VI

Chair: Tymish Y. Ohulchanskyy

16:30	**Junle Qu** (Shenzhen, China) Advancing biomedical optical imaging: breakthroughs in superresolution, multimodal, and deep-tissue microscopy	p. 35
17:00	**Michal Nowakowski** (Paderborn, Germany) Charge transfer in base metal dyad evidenced by fs-XES	p. 36
17:30	**Magdalena Jaglarz** (Kraków, Poland) Radiation protection at SOLARIS National Synchrotron Radiation Centre	p. 37
17:45	**Zofia Borowska** (Paderborn, Germany) Noble metal-based catalyst for NO_x reduction	p. 38

Invited talk, Thu./16:30

Advancing biomedical optical imaging: breakthroughs in superresolution, multimodal, and deep-tissue microscopy

J. Qu

Center for Biomedical Photonics, College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen 518060, China

email: `jlqu@szu.edu.cn`

Optical microscopy is crucial for understanding biological processes and advancing clinical diagnostics, but its limitations prevent it from reaching its full potential. Diffraction restricts resolution, light scattering reduces imaging depth and accuracy in thick tissues, and single-modality approaches fail to provide comprehensive functional information. To address these challenges, we propose a range of innovative strategies to enhance spatial and temporal resolution, imaging depth, and multimodal capabilities. These advancements include: (1) super-resolution imaging using stimulated emission depletion (STED) and fluorescence spatial-temporal modulation (FSTM), achieving nanoscale resolution for tracking subcellular dynamics; (2) deep-tissue imaging leveraging adaptive optics, near-infrared probes, and multiphoton excitation to minimize light scattering and enable high-resolution visualization in living systems; and (3) the development of multimodal platforms that integrate laser scanning confocal microscopy and wide-field microscopy across visible and near-infrared wavelengths. These platforms combine two-photon excited fluorescence (TPEF), second harmonic generation (SHG), and fluorescence lifetime imaging (FLIM) to correlate structural, functional, and molecular information. These technologies have been successfully applied in biomedical research, including real-time monitoring of organelle activity and the early diagnosis of neuropathologies. Future directions include incorporating artificial intelligence to enhance the flexibility and precision of super-resolution imaging, as well as refining in vivo multimodal imaging to reduce phototoxicity and achieve more accurate diagnoses. By aligning technological innovation with biomedical needs, our work promotes the development of accessible, high-precision optical tools that can transform research and healthcare.

Acknowledgements: We acknowledge the support of the National Key R&D Program of China, the National Natural Science Foundation of China, and the Shenzhen Science and Technology Program.

[1] L. Wang *et al.*, Light Sci. Appl., 14 (2025), 32
[2] J. Qu *et al.*, Anal. Chem., 96 (2024), 2754-2758

INVITED TALK, THU./17:00

Charge transfer in base metal dyad evidenced by fs-XES

M. Nowakowski and M. Bauer

Fakultät für Naturwissenschaften, Universität Paderborn, Warburger Str. 100, 33098 Paderborn, Germany

email: `michal.nowakowski@upb.de`

The photocatalytic proton reduction using sunlight allows production of molecular hydrogen in a sustainable way [1]. Fe(II) complexes are one example of prototypical earth-abundant and biocompatible photosensitizers for this purpose [2]. Metal-to-ligand charge transfer (MLCT) lifetimes in Fe(II) complexes with N-heterocyclic carbene ligands (NHC) are sufficiently long for direct electron transfer to a water reduction catalyst in bimetallic dyads and initiating the photoinduced redox process.

The model Fe-Co system is shown in Figure 1 A and consists of Fe(II)-NHC photosensitizer (PS) connected covalently to the cobaloxime catalyst. As the involved states at the cobalt center are known to be optically dark [3], the full electron dynamics can only be studied with atomic- and state-focused techniques. We investigated electron dynamics upon 400 nm excitation on Fe and Co K-edges simultaneously using femtosecond Kα XES at FXE beamline at European XFEL. We found a complicated excited state cascade with the MLCT state at Fe(II) moiety living up to 10-12 ps and a charge transfer from it to the [Co] part (Figure 1 B). The Fe(II) catalyst exhibited nuclear wavepacket dynamics, different in PS and Fe-Co systems. With multiplet and CASSCF calculations we described the full excited state structure of the complex [3].

The knowledge of the dyad's excited state landscape pointed out the critical vectors for improvement of the system. As prototypic, yet catalytically active complex, this opens a field for a new approach to sustainable H_2 production.

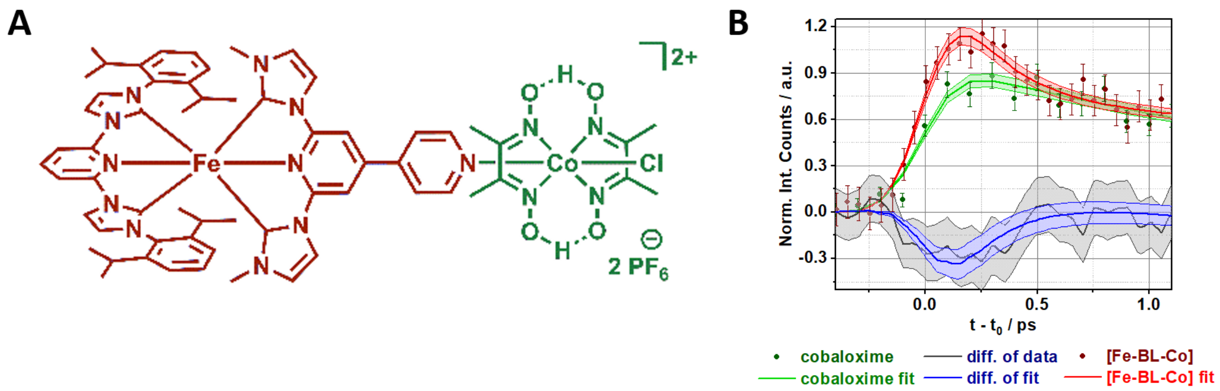

Figure 1: A) Structure of the dyad: photosensitizer (red) and cobaloxime (green); B) Dynamic charge transfer signature in [Co] moiety of the dyad.

Acknowledgements: The authors acknowledge European XFEL in Schenefeld, Germany, for the provision of X-ray free-electron laser beamtime at FXE and would like to thank the instrument group and facility staff for their expert assistance. M.B. acknowledges funding by the German DFG in the frame of priority program SPP 2102 (Grant number BA 4467/7-1) and the German BMBF (Grant numbers 05K19PP1 and 05K18PPA). Generous grants of computer time at the Paderborner Center for Parallel Computing PC^2 are gratefully acknowledged.

[1] P. Zimmer *et al.*, Eur. J. Inorg. Chem., 2017 (2017), 1504-1509
[2] Y. Liu *et al.*, Acc. Chem. Res., 49 (2016), 1477-1485
[3] M. Nowakowski *et al.*, Adv. Sci., 11 (2024), 2404348

Contributed talk, Thu./17:30

Radiation protection at SOLARIS National Synchrotron Radiation Centre

M. Jaglarz, A. Toboła-Galus, and D. Raś

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

email: `magdalena.jaglarz@uj.edu.pl`

From the perspective of radiation protection, the National Synchrotron Radiation Centre SOLARIS, as the first synchrotron in Poland, must explore dedicated strategies to adhere to the requirements outlined in the Atomic Law. The facility specificity, which operates high-energy accelerator systems and associated beamlines and simultaneously provides infrastructural access to hundreds of researchers yearly, demands dedicated procedures and high-tech systems to monitor radiation levels in the facility continuously. Further, the radiation protection solutions must be coordinated in accordance with the other relevant safety rules, including daily use of the facility, maintenance works around accelerator tunnels, or chemistry and biological risks associated with the materials brought by the users.

Since the beginning of operation in 2015, radiation levels within the facility have been measured using radiation monitoring stations (RMS), thermoluminescent dosimeters (TLDs), and portable radiometers [1]. Additionally, radiation exposure is monitored through individual thermoluminescent dosimeters (TLDs) and, when required, electronic dosimeters [2]. Furthermore, the research infrastructure at SOLARIS includes a Personal Safety System (PSS) designed to protect personnel and users from ionizing radiation. This system controls access to restricted areas and automatically stops operations in case of hazardous situations.

In the presentation, we will discuss the SOLARIS infrastructure from the perspective of radiological protection, with a particular focus on the efficiency, readiness, feedback loops, and signal correlations of the devices installed on-site to maintain constant radiation monitoring and safe user operation.

Acknowledgements: This project is developed under the provision of the Polish Ministry and Higher Education project “Support for research and development with the use of research infrastructure of the National Synchrotron Radiation Centre SOLARIS” under contract nr 1/SOL/2021/2.

[1] M. B. Jaglarz *et al.*, “Radiation safety at Solaris 1.5 GeV storage ring” IPAC2019, Melbourne, Australia, JACoW Publishing doi:`10.18429/JACoW-IPAC2019-THPRB059`

[2] M. B. Jaglarz *et al.*, „Radiation Protection and Personal Safety System at SOLARIS National Synchrotron Radiation Centre” Radsynch23, 11th International on Radiation Safety at Synchrotron Sources, ESRF-Grenoble-France, 30 May - 2 June 2023

Contributed talk, Thu./17:45

Noble metal-based catalyst for NO_x reduction

Z. I. Borowska[1], Ö. Selcuk[2], R. Schoch[1], S. Kureti[2], and M. Bauer[1]

[1] *Universität Paderborn, Warburger Str. 100, 33098 Paderborn, Germany*
[2] *Technische Universität Bergakademie Freiberg, Akademiestr. 6, 09599 Freiberg, Germany*

email: `zofia.borowska@upb.de`

To decrease the emission of toxic nitrogen oxides (NO_x) from engines [1], hydrogen is used for O_2-rich and low-temperature NO_x reduction in exhaust gas (H_2-deNO_x). Current methods are low-efficient and low-selective towards the aimed N_2. Instead, we propose a catalyst based on Pt doped with W/Mo as an electronic promotor supported on ZrO_2 (Pt@WO_x/MoO_xZrO_2). The aim of this study is to determine the influence of the W/Mo addition on the performance and structure of the catalyst under reaction conditions and the reaction mechanism.

The reaction was performed on the Pt@WO_x/MoO_xZrO_2 catalyst to study its activity and selectivity. TEM and Raman spectroscopy were used to study the catalyst's structure, as well as XPS, the reactants' adsorption on the surface. Due to the elemental specificity and the electronic and structural sensitivity, XAS will be used to determine the influence of the W/Mo addition on the structure of the catalyst in the reaction.

Reaction performance results on the Pt@WO_x/MoO_xZrO_2 indicate high conversion and N2-selectivity at low temperatures (Fig.1a,b) [2]. In the Pt@WO_xZrO_2 bulk structure (TEM), however at high W loading the crystal structure and metallic Pt was revealed (Raman spectroscopy, XPS). Similarly, in the Pt@MoO_xZrO_2, the structure was determined to crystalize with rising Mo loading [2]. XPS results indicate the reaction mechanism (H_2 adsorption). XAS experiments will provide the Pt oxidation state, structural effects (agglomeration), and the possible correlation of the W/Mo addition to the catalyst's structure.

The results give an insight into the influence of W/Mo addition on the structure and performance of the catalyst and the reaction mechanism. This information leads towards the effective systems for the NO_x reduction in exhaust gas.

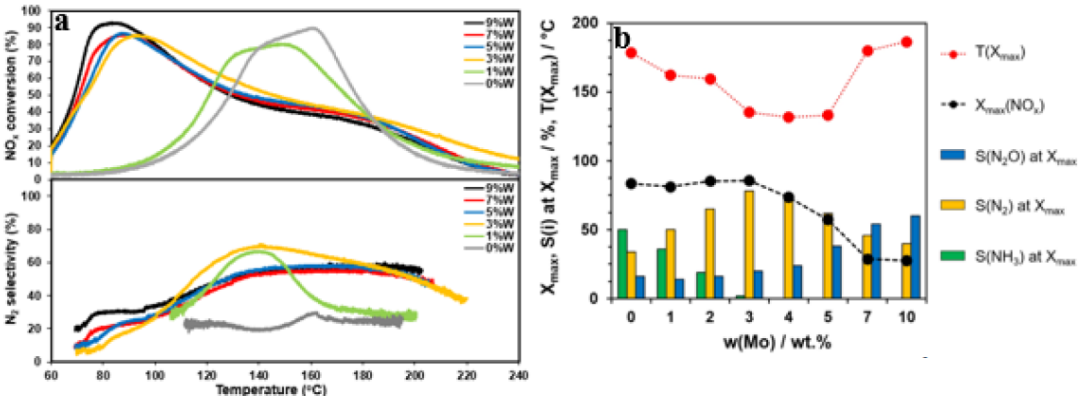

Figure 1: Reaction performance of the a. Pt@WO_xZrO_2 and b. Pt@MoO_xZrO_2 catalyst

[1] European Environment Agency (EEA) (2024). (`https://doi.org/10.2908/ENV_AIR_GGE`)
[2] D. Schröder and S. Kureti, Top. Cat., 66 (2023), 787-796

SESSION VII

Chair: Ryszard Sobierajski

09:00	**Serguei Molodtsov** (Schenefeld, Germany) European XFEL: Properties of FEL radiation and its main areas of application	p. 40
09:30	**Przemysław Nogły** (Kraków, Poland) Time-resolved serial crystallography at synchrotrons and XFELs	p. 41
10:00	**Wojciech Błachucki** (Kraków, Poland) Study on the two-color X-ray pulses at SwissFEL	p. 42

INVITED TALK, FRI./09:00

European XFEL: Properties of FEL radiation and its main areas of application

S. L. Molodtsov

European XFEL, Holzkoppel 4, 22869 Schenefeld, Germany

email: `serguei.molodtsov@xfel.eu`

The European X-ray Free Electron Laser (XFEL) is a new international research installation that is under 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, pharmaceutics, 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 present 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 (200 as - 100 fs) that makes the facility particular suitable for time-resolved X-ray absorption, photoemission, (resonance) inelastic X-ray scattering as well as diffraction and imaging studies in the range of moderate and hard X-ray photons.

In this talk an overview of the European XFEL project, properties of FEL radiation as well as its main areas of application will be presented.

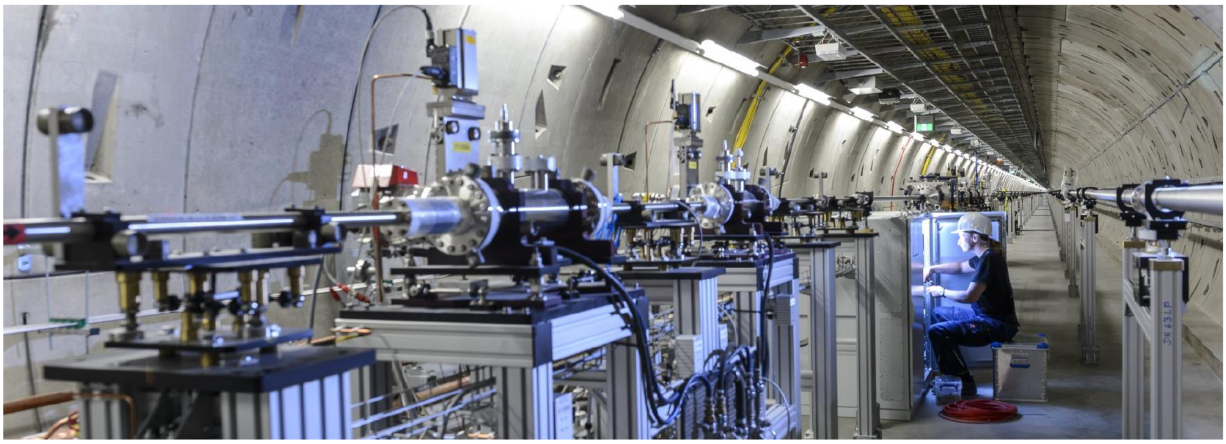

Figure 1: European XFEL beamline.

INVITED TALK, FRI./09:30

Time-resolved serial crystallography at synchrotrons and XFELs

P. Nogly

Dioscuri Centre for Structural Dynamics of Receptors, Faculty of Biochemistry, Biophysics and Biotechnology, Jagiellonian University, Kraków, Poland

email: `przemyslaw.nogly@uj.edu.pl`

Chloride transport is an essential process maintaining ion balance across cell membranes, cell growth, and neuronal action potentials. However, the molecular mechanism of the transport remains elusive. Among chloride transporters, light-driven rhodopsins have gained attention as optogenetic tools to manipulate neuronal signaling. We combined time-resolved serial crystallography (SwissFEL and SLS synchrotron) to provide a comprehensive view of chloride-pumping rhodopsin's structural dynamics and molecular mechanism throughout the transport cycle from 10 ps to 50 ms [1]. We traced transient anion binding sites, obtained evidence for the mechanism of light energy utilization in transport, and identified steric and electrostatic molecular gates ensuring unidirectional transport. These structural insights provided the basis for mutagenesis and functional study of the mechanistic features enabling finely controlled chloride transport across the cell membrane.

Furthermore, I will present insights into the photochemistry and selectivity of retinal isomerization in proton-pumping rhodopsin [2] and show that, in favorable cases, even larger structural changes can be captured in crystals [3].

Our recent study of a distinct photoreceptor, Light-Oxygen-Voltage (LOV) domain, will be introduced. The first insights into the structural dynamics of LOV photoactivation will be presented, providing the basis for proposing a molecular mechanism of a covalent thioether bond formation between a flavin mononucleotide cofactor and a reactive cysteine, Cys57 (unpublished).

Acknowledgements: The project was financed under Dioscuri, a program initiated by the Max Planck Society, jointly managed with the National Science Centre in Poland, and mutually funded by the Polish Ministry of Education and Science and the German Federal Ministry of Education and Research. This research was funded by the National Science Centre, grant agreement No. UMO-2021/03/H/NZ1/00002. We also acknowledge infrastructural support by the Strategic Programme Excellence Initiative at Jagiellonian University - BioS PRA. The project was initiated with funding received from the Swiss National Science Foundation Ambizione grant PZ00P3_174169.

[1] S. Mous *et al.*, Science, 375 (2022), 845
[2] P. Nogly *et al.*, Science, 361 (2018), eaat0094
[3] T. Weinert *et al.*, Science, 365 (2019), 61

INVITED TALK, FRI./10:00

Study on the two-color X-ray pulses at SwissFEL

W. Błachucki[1], P. Dijkstal[2], E. Prat[2], C. Vicario[2], and C. Arrell[2]

[1]*Institute of Nuclear Physics, Polish Academy of Sciences, 31-342 Kraków, Poland*
[2]*Paul Scherrer Institute, 5232 Villigen, Switzerland*

email: `wojciech.blachucki@ifj.edu.pl`

Recently, X-ray pump-X-ray probe experiments have become a significant area of focus. These experiments allow researchers to specifically excite parts of a molecule or an electron shell within an atom using an initial X-ray pulse (the pump) and then observe its subsequent changes with a second X-ray pulse (the probe). To overcome the problem of timing inconsistencies when using two independent X-ray sources, various X-ray free-electron lasers (XFELs) are developing a "two-color" method. This technique generates two distinct X-ray pulses from a single electron bunch. At SwissFEL, this two-color operation is achieved by using a short ultraviolet (UV) pulse that overlaps with the photocathode drive laser used to generate the electron bunch [1]. This UV pulse increases the spread of the electron bunch in a specific time window. This increased spread hinders the free-electron laser process in that region, resulting in the creation of two separate X-ray subpulses instead of a single one.

In this study, SwissFEL operated in this two-color mode, produced X-ray pulses with an average energy of 570 µJ. Each pulse contained two energy components: one at 6937 eV and another at 6978 eV, with an energy difference of 41 eV. The time difference between these two energy components within each X-ray pulse was measured using a THz streaking setup. This measurement was then compared to the electron bunch's time structure, which was analyzed using a passive streaker located after the undulator section. The time delay measured with the THz streaking method was found to be approximately 1.5 to 3.0 times larger than the 60 fs delay indicated by the passive streaker measurement.

Acknowledgements: W.B. acknowledges the National Science Centre (Poland) for financial support under the grant of number 2019/03/X/ST2/00949.

[1] C. Vicario *et al.*, Phys. Rev. Accel. Beams, 24 (2021), 060703

SESSION VIII

Chair: Przemysław Nogly

11:30	**Wojciech Gawelda** (Madrid, Spain) Photoinduced structural changes in Cu-prion peptide complex studied by ultrafast X-ray techniques	p. 44
12:00	**Ryszard Sobierajski** (Warsaw, Poland) Scientific opportunities at XFEL	p. 45
12:30	**Mohammad Sadegh Shakeri** (Kraków, Poland) Pulsed laser irradiation of colloids: insights from experiments and theory	p. 46

INVITED TALK, FRI./11:30

Photoinduced structural changes in Cu-prion peptide complex studied by ultrafast X-ray techniques

W. Gawelda[1,2,3]

[1]Department of Chemistry, Universidad Autónoma de Madrid, 28049 Madrid, Spain
[2]IMDEA Nanoscience, 28049 Madrid, Spain
[3]Faculty of Physics, Adam Mickiewicz University, 61-614 Poznań, Poland

email: `wojciech.gawelda@amu.edu.pl`

The cellular prion protein (PrP^C) is a membrane-bound glycoprotein and has emerged as an important copper binding protein. It is known that the redox behavior of Cu bound to PrP^C, plays an important role in both the physiological function of the protein, and in the pathogenesis of neurodegenerative diseases known as prion diseases. They are accompanied by an accumulation of a misfolded and non-soluble isoform of PrP^C [1]. NMR studies on human PrP^C demonstrate that the C-terminal region (Fig 1A), which adopts a globular fold that is largely helical, and the N-terminal region, which is unstructured and flexible in solution [2]. A hallmark of this region is the so-called octa-repeat (OR) domain, which has a strong affinity to Cu^{2+} ions [3]. There is evidence that the OR domain can reduce Cu^{2+} via an electron transfer (ET) from a tryptophan (Trp) residue. DFT and MD simulations demonstrated that the resulting Cu(I) and reactive oxygen species can lead to formation of the precursor of the pathogenic PrP^C structures.

Up to date, no direct measurement of Trp*-Cu^{2+} ET and the structural changes accompanying it has been reported. Here we mimic the biological activity by photoexciting a Trp residue present in the N-terminal region of the protein (Fig. 1B). Preliminary time-resolved results obtained using X-ray free electron lasers are shown in Figs 1C-D. We have used a combination of fs-XAS and X-ray scattering to track ET process involving Cu^{2+} active site and the subsequent structural changes of the nearby environment upon photoreduction.

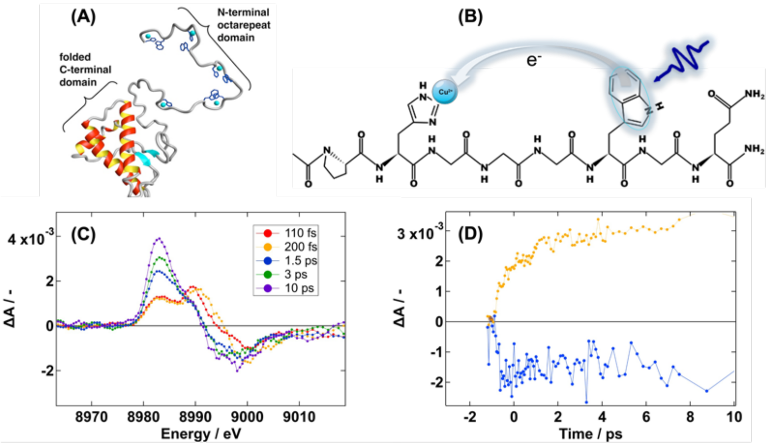

Figure 1: (A) PrP^C structure indicating the positions of Cu^{2+} sites; (B) OR-Cu^{2+} complex showing the photoexcitation mechanism leading to an ET from Trp towards Cu^{2+} site; (C) Transient XAS at Cu K-edge at selected time delays; (D) Spectral kinetics at selected X-ray photon energies shown in (C).

[1] S.B. Prusiner, PNAS, 95 (1998), 13363
[2] R. Zahn *et al.*, PNAS, 97 (2000), 145
[3] L. Quintanar *et al.*, Coord. Chem. Rev., 257 (2013), 429-444

Invited talk, Fri./12:00

Scientific opportunities at XFEL

R. Sobierajski[1], W. Gawełda[2], A. Glinka[2], K. Jarzembska[3], R. Kamiński[3], M. Kozak[2], J. Kubicki[2], and D. Milewska[4]

[1] *Institute of Physics Polish Academy of Sciences, al. Lotników 32/46, 02-668 Warsaw, Poland*
[2] *Faculty of Physics, Adam Mickiewicz University, ul. Uniwersytetu Poznańskiego 2, 61-614 Poznań, Poland*
[2] *Department of Chemistry, University of Warsaw, Żwirki i Wigury 101, 02-089 Warsaw, Poland*
[2] *National Centre for Nuclear Research, ul. Andrzeja Sołtana 7, 05-400 Otwock-Świerk*

email: `ryszard.sobierajski@ifpan.edu.pl`

The European X-ray Free Electron Laser (EuXFEL) is an international laboratory where intense ultrashort pulses X-rays are generated and applied in scientific research. It contributes to the significant expansion of our knowledge in many scientific disciplines (m.in. medicine, pharmacology, chemistry, materials science, nanotechnology, energy and electronics) and the emergence of new technologies affecting our daily lives. During the presentation, a Project financed by the Ministry of Science and Higher Education to support the Polish scientific community in the use of new research opportunities offered by EuXFEL will be presented [1]. The project includes the following activities:

1. training in basic knowledge of XFEL applications and research techniques used, including several months of internships for young researchers at institutions participating in XFEL research and a lecture on XFEL for undergraduate and doctoral students;
2. funding the participation of Polish scientists in conferences and workshops on XFEL research;
3. assistance in establishing or expanding scientific contacts with EuXFEL employees and/or research groups carrying out similar research in Poland and abroad;
4. assistance in the preparation of research projects in competitions for measurement time on XFEL sources, also by performing pilot and complementary studies.

The lecture will end with a presentation by the Network of Centres of Excellence in the field of research using XFEL (CD XFEL), in which the above program is implemented.

Acknowledgements: Co-financed by the Ministry of Science and Higher Education program "Support for the participation of Polish research teams in international research infrastructure projects", based on contract No. 2022/WK/13.

[1] `www.ifpan.edu.pl/cd-xfel`

Contributed talk, Fri./12:30

Pulsed laser irradiation of colloids: insights from experiments and theory

M. S. Shakeri and Ż. Swiątkowska-Warkocka

Institute of Nuclear Physics Polish Academy of Sciences, PL-31342 Krakow, Poland

email: `ms.shakeri@ifj.edu.pl`

This presentation explores the use of pulsed laser irradiation of colloidal nanoparticles as an innovative method for synthesizing heterostructure particles. The process involves irradiating transition metals and their oxides, where physical perturbations in the colloidal environment drive chemical phase formation, resulting in variable oxidation states and highly active surfaces [1]. These unique properties make the synthesized particles exceptionally suited for surface-dependent applications such as catalysis. The talk will highlight experimental findings, focusing on how microstructural transformations can be controlled by tuning synthesis parameters [2]. Insights into oxidation state variations will be presented, with a particular emphasis on synchrotron-based characterization techniques. Additionally, theoretical support through ab-initio subatomic calculations and atomistic simulations will be discussed, providing a deeper understanding of the experimental observations. In the concluding section, the application of the synthesized heterostructures in ethanol oxidation reactions within electrocatalytic fuel cells will be addressed, showcasing their potential in renewable energy technologies [1].

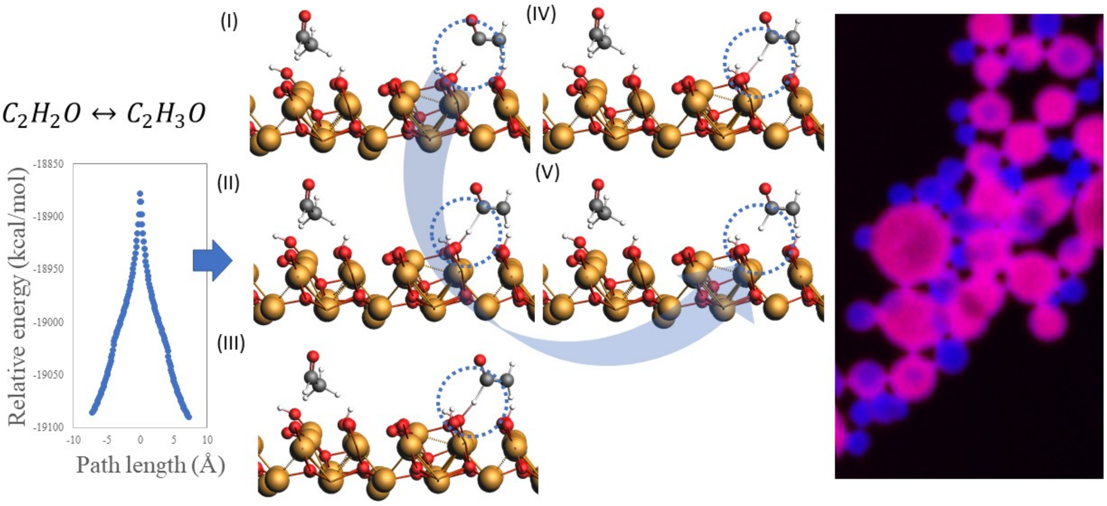

Figure 1: Basin-hopping local minima exploration and kinetics of bond formation during solvent absorption. The creation of core-shell structure after pulsed laser irradiation of colloids.

Acknowledgements: This work was supported by the Polish National Science Centre, Programs No. 2022/06/X/ST3/01743 and 2018/31/B/ST8/03043. Part of the computational work was conducted in collaboration with the Prometheus Cluster at Cyfronet, AGH University of Science and Technology, Krakow, utilizing Grant No. PLG/2022/015573.

[1] M. S. Shakeri *et al.*, Adv. Funct. Mater., 33 (2023), 2304359
[2] M. S. Shakeri *et al.*, Sci. Rep., 12 (2022), 11950

SESSION IX

Chair: Edyta Piskorska - Hommel

14:00	**Erik Čižmár** (Košice, Slovakia) Cluster spin glass in layered double hydroxides	p. 48
14:30	**Christopher J. Stanton** (Gainesville, USA) Manipulating g-factors, spin, and effective masses in semiconductor nanostructures	p. 49
15:00	**Jędrzej Kobylarczyk** (Kraków, Poland) Temperature and solvent vapors switchable molecular clusters	p. 50
15:15	**Illia Kozin** (Košice, Slovakia) Magnetic properties of the 2D Heisenberg quantum magnet $Cu[C_6H_2(COO)_4][H_2(CH_3NH)_2C_2H_4]$ on rectangular lattice	p. 51
15:30	**Anna Nykiel** (Kraków, Poland) The evolution of magnetic behavior in FeCoNi nanowires with different geometry	p. 52

INVITED TALK, FRI./14:00

Cluster spin glass in layered double hydroxides

E. Čižmár[1], V. Tkáč[1], E.L. Fertman[2], A.V. Fedorchenko[2], Yu.G. Pashkevich[3,4], M. Holub[5], R. Tarasenko[1], A. Feher[1], C.S. Neves[6], D.E.L. Vieira[6], and A.N. Salak[6]

[1]*Institute of Physics, Faculty of Science, P.J. Šafárik University in Košice, 04154 Košice, Slovakia*
[2]*B. Verkin Institute for Low Temperature Physics and Engineering of NASU, 61103 Kharkiv, Ukraine*
[3]*O. Galkin Donetsk Institute for Physics and Engineering of NASU, 03028 Kyiv, Ukraine*
[4]*Department of Physics and Fribourg Center for Nanomaterials, University of Fribourg, CH-1700 Fribourg, Switzerland*
[5]*Synchrotron SOLEIL, L'Orme des Merisiers, St Aubin BP48, Gif sur Yvette Cedex 91192, France*
[6]*Department of Materials and Ceramics Engineering, CICECO - Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal*

email: `erik.cizmar@upjs.sk`

Frequency-dependent magnetic behaviour of Co-Al layered double hydroxides (LDH) with the Co/Al ratio (n) of 2 and 3, and the basal spacing values in the range of 0.76-1.66 nm was studied in detail between 2 and 300 K. It was found from analysis of the temperature-dependent *ac* magnetic susceptibility measured at different frequencies that the studied LDH exhibit a magnetic cluster spin glass (spin glass-like) behaviour regardless of their basal spacing value and the Co/Al ratio as evidenced by $E_A/k_BT_0 > 1$ relation as obtained from the analysis using Vogel-Fulcher law [1]. The obtained values of Mydosh parameters in the range of 0.017-0.052 suggest that some of these materials are not far from the canonical spin glasses, implying a rather small size of the magnetic clusters. Unlike in Co-Al LDH with low freezing temperatures, Ni-Fe LDH display a glassy state at higher temperatures, which could enable the study of aging and memory effects in spin glasses.

The specific heat of non-magnetic Mg-Al LDH at low temperatures temperatures revealed their 2D solid and structural glass character [2]. The reduced $C(T)/T^3$ of Mg-Al LDH intercalated with nitrate was found to demonstrate a so-called boson peak, which is a manifestation of a glassy state. The observed low-temperature structural glassy state in LDH was associated with the disorder of the intercalated species and can affect the creation of cluster spin glass in magnetic LDH.

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

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

Invited talk, Fri./14:30

Manipulating g-factors, spin, and effective masses in semiconductor nanostructures

C. J. Stanton

Department of Physics, 2001 Museum Road, P.O. Box 118440, University of Florida, Gainesville, Florida, 32611-8440 USA

email: `stanton@ufl.edu`

The ability to engineer and manipulate g-factors and hence the spin in semiconductor nanostructures is important for a wide variety of novel spintronic applications. In this talk, we look at g-factor engineering in narrow gap $\mathrm{InAs}_x\mathrm{P}_{1-x}$ nanostructures. $\mathrm{InAs}_x\mathrm{P}_{1-x}$ alloys are important for device applications since the band gaps can vary from 0.36 eV (InAs) to 1.35 eV (InP) covering ∼3.4 mm to 900 nm (mid to near infrared). In addition $\mathrm{InAs}_x\mathrm{P}_{1-x}$ offers a wide tunability of the g-factor ranging from 1.2 for InP to -14.75 for InAs and even higher if doped with magnetic impurities. The sign change in the g-factor offers the intriguing possibility of creating an alloy with a zero g-factor, important for photodetectors for quantum information and sensing. To preserve the entanglement one needs a material that has a conduction band effective g-factor much smaller than the valence band so that the photodetector can excite equally to the spin split states. In this work, we studied the magneto-optical properties of $\mathrm{InAs}_x\mathrm{P}_{1-x}$ films and nanostructures at ultrahigh magnetic fields (up to 120 T). We investigated how one can change and manipulate the g-factors and effective masses with: 1) quantum confinement, 2) magnetic impurities such as Mn, 3) magnetic fields, and 4) alloying. Our results show[1] that a g-factor close to zero can be achieved in $\mathrm{InAs}_x\mathrm{P}_{1-x}$ with an alloy concentration x slightly less than 0.34. This fact introduces the prospects of using these materials system for quantum communication devices and g-factor engineering.

Acknowledgements: This work was supported by the AFOSR through grant FA9550-24-1-0059.

[1] S. K. Thapa *et al.*, Phys. Rev. B, 108 (2023), 115202

Contributed talk, Fri./15:00

Temperature and solvent vapors switchable molecular clusters

J. Kobylarczyk[1], L. Shi[2, 3], and R. Podgajny[2]

[1]*Institute of Nuclear Physics Polish Academy of Sciences, Kraków, Poland*
[2]*Faculty of Chemistry, Jagiellonian University, Kraków, Poland*
[3]*Department of Chemistry, Zhejiang University, Hangzhou, China*

email: `jedrzej.kobylarczyk@ifj.edu.pl`

Multifunctional molecular materials based on coordination polynuclear multi-site molecules lie at the heart of materials sciences in view of growing technological challenges dedicated to the progressive miniaturization process in information processing and storage as well as sensor devices. Invariably particular interest in research is focused on molecular materials combining several desirable physicochemical properties to conform switchability regime, and thus, to constituting the physical basis for recording, reading, and processing information. In this context, one of the perfect candidates for our consideration are molecular compounds with two or more inequivalent spin states, which could be switched by convenient external stimulus such as temperature, light, electric current, sorption/desorption of vapors or chemical activation. [1]

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

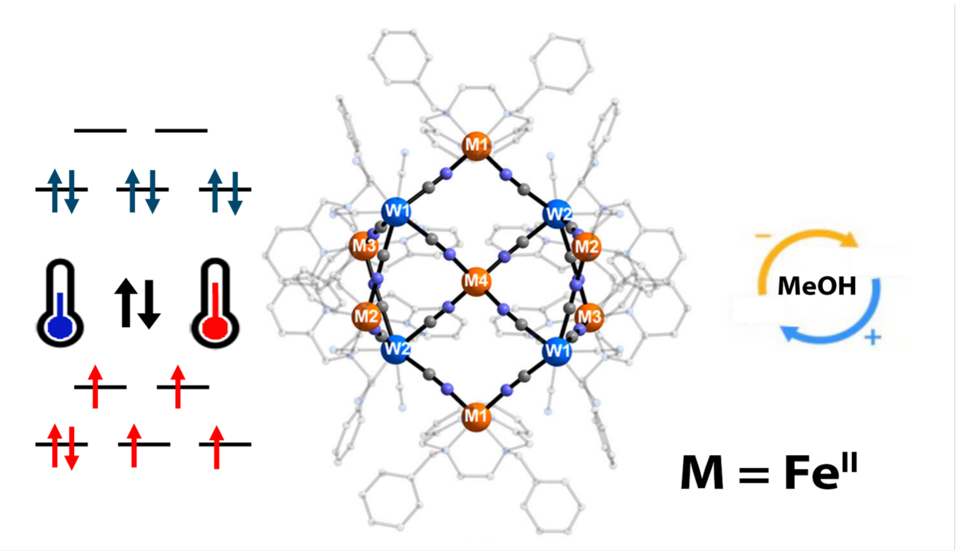

Figure 1: Coordination skeleton of $\{Fe^{II}[Fe^{II}(bzbpen)]_6[W^{V}(CN)_8]_2[W^{IV}(CN)_8]_2\}$ cluster

[1] J. Kobylarczyk *et al.*, Coord. Chem. Rev., 419 (2020), 213394
[2] L. Shi *et al.*, Inorg. Chem., 62 (2023), 7032

Contributed talk, Fri./15:15

Magnetic properties of the 2D Heisenberg quantum magnet $Cu[C_6H_2(COO)_4][H_2(CH_3NH)_2C_2H_4]$ on rectangular lattice

I. Kozin, R. Tarasenko, V. Tkáč, A. Orendáčová, E. Čižmár, and M. Orendáč

Institute of Physics, Faculty of Science, P. J. Šafárik University, Park Angelinum 9, 040 01 Košice, Slovakia

email: `illia.kozin@student.upjs.sk`

Copper (II)-based magnets exhibit unique physical properties as a result of quantum spin phenomena and the low-dimensionality of their magnetic subsystem. An experimental study of the thermal and magnetic properties of a novel metal-organic complex $Cu[C_6H_2(COO)_4][H_2(CH_3NH)_2C_2H_4]$ is presented, where Cu^{2+} ions, together with pyromellitic acid anions $[C_6H_2(COO)_4]^{4-}$, create a framework of 2D magnetic layers, which are shifted by the cations of the organic compound *dmeda* - $[H_2(CH_3NH)_2C_2H_4]^{2+}$.

Specific heat measurements of powder sample over the temperature range from 0.38 K to 30 K and magnetic fields up to 9 T were performed in a commercial PPMS device equipped with ^{3}He insert. The zero-field data showed reasonable agreement with a theoretical model for 2D Heisenberg antiferromagnet on a rectangular lattice, characterized by spatial anisotropy parameter $R = 0.45$ with antiferromagnetic exchange interaction $J/k_B \approx 9.47$ K. Additionally, zero-field heat capacity exhibit no magnetic phase transition to long range order down to 0.38 K, although the in-field data clearly indicate the presence of a field-induced Berezinskii-Kosterlitz-Thouless transition.

Magnetization temperature dependences were measured in a Quantum Design MPMS magnetometer in the temperature range from 1.8 to 300 K in magnetic field of 100 mT. The low-temperature susceptibility analysis yielded not only g-factor to be around 2.02, but also the same value of $R = 0.45$, while $J/k_B \approx 9.2$ K was found to be slightly lower in comparison with heat capacity data. Furthermore, $g = 2.02$ was confirmed by Curie-Weiss and effective magnetic moment analysis. The analysis of specific heat, magnetic susceptibility and magnetization identified the studied compound $Cu[C_6H_2(COO)_4][H_2(CH_3NH)_2C_2H_4]$ as a quasi-two-dimensional $S = 1/2$ Heisenberg antiferromagnet on the rectangular lattice.

Acknowledgements: The financial support of projects VEGA 1/0132/22, APVV-18-0197, APVV-22-0172 and APVV-23-0006 is acknowledged.

Contributed talk, Wed./15:30

The evolution of magnetic behavior in FeCoNi nanowires with different geometry

A. Nykiel[1], A. Zarzycki[1], W. Maziarz[2], J. Ghanbaja[3], A. Walcarius[3], and M. Kac[1]

[1]*Institute of Nuclear Physics, Polish Academy of Sciences, PL-31-342 Kraków, Poland*
[2]*Institute of Metallurgy and Materials Science, Polish Academy of Sciences, PL-30-059 Kraków, Poland*
[3]*Lorraine University, CNRS, F-54000 Nancy, France*

email: `anna.nykiel@ifj.edu.pl`

Nanoscale materials, especially nanowires (NWs), which are defined as one-dimensional objects, are attractive for a wide range of applications and fundamental studies. Among nanowires, the magnetic structures, whose properties are strongly dependent on their geometry, deserve special attention. Such nanowires can be relatively easily obtained using the template-assisted electrodeposition method.

Thus, in this work, we studied FeCoNi nanowires electrodeposited in polycarbonate membranes as a function of their lengths and diameters. The nucleation mechanism investigated for nanowires with smaller diameters (up to 100 nm) suggested the progressive type and evolved to instantaneous nucleation for larger ones. The studies of NW morphology revealed twinning defects that appeared in all samples independent of their geometry. The chemical composition analysis, unaffected by NW dimensions, indicated 13% Fe, 24% Co, and 63% Ni. Changes in the geometry resulted in the modification of the coercivity and squareness, increasing with the decrease in nanowire diameter and length. Studies of the reversal mechanism showed a non-monotonic coercivity variation as a function of angle, suggesting an initial propagation of the vortex domain wall that transformed into a transverse or coherent rotation. FORC analysis designated a non-interacting system in the case of a small diameter NW matrix, confirming that the nanowire diameter is the main factor determining magnetostatic interaction between nanowires. Magnetic imaging of the sample using Lorentz microscopy did not reveal a domain structure, which points out a single-domain structure of nanowires.

SESSION X

Chair: Christopher Stanton

16:30	**Suja Elizabeth Saji** (Bangalore, India) Tuning spin reorientation and switching transitions in rare-earth orthoferrite crystals	p. 54
17:00	**Edyta Piskorska-Hommel** (Wrocław, Poland) Molecular beam epitaxy: principles, techniques, and advanced applications	p. 55
17:30	**Artur Glavic** (Villigen, Switzerland) Studying magnetic nanomaterials using neutron scattering	p. 56
18:00	**Sajid Sekh** (Kraków, Poland) Topological in-gap chiral edge states in superconducting Haldane model with spin-orbit coupling	p. 57

INVITED TALK, FRI./16:30

Tuning spin reorientation and switching transitions in rare-earth orthoferrite crystals

S.E. Saji

Department of Physics, Indian Institute of Science, Bangalore-560012, India

email: `liz@iisc.ac.in`

Rare-earth orthoferrite, $RFeO_3$ compounds exhibit unique properties such as spin reorientation transitions (SRT), spin switching (SSW), ultrafast spin dynamics, and long-range spin transport. These materials display antiferromagnetic Fe^{3+} spin ordering below 650-760 K, accompanied by weak ferromagnetic moments (WFM) induced by Dzyaloshinskii-Moriya (DM) interactions. The WFM aligns along the a-axis in the Γ_2 phase and the c-axis in the Γ_4 phase and is absent in the Γ_1 phase. For R=Pr, Nd, Sm, Tb, Ho, Er, Tm, and Yb, an SRT from Γ_4 to Γ_2 occurs upon cooling, while $CeFeO_3$ and $DyFeO_3$ transform to Γ_1 phase. Exchange interactions between Fe^{3+} and R^{3+} ions drive SRT, while SSW, characterized by flipping magnetic moments due to Fe and R spin reversal, manifests in compounds such as $NdFeO_3$, $SmFeO_3$, and $ErFeO_3$. Rare-earth ions are critical for SSW, which arise when their polarization opposes the Fe WFM. External magnetic fields can tune the spin-switching temperature (T_{SSW}).

I will discuss spin reorientation and switching transitions in $RFeO_3$ single crystals investigated through Magnetization measurements. A series of high-quality single crystals of $Er_{1-x}Sm_xFeO_3$ (x=0, 0.2, 0.4, 0.6, 0.8) were grown using the optical floating zone method. Structural and preliminary characterizations confirmed the phase purity and quality of the crystals. Rietveld refinement of powder XRD data revealed systematic changes in a and c lattice parameters with increasing Sm content. Magnetization measurements under field-cooled cooling (FCC) conditions showed a temperature-induced spin-reorientation transition (SRT) from $\Gamma_4(G_x, A_y, F_z)$ to $\Gamma_2(F_x, C_y, G_z)$ across all compositions, with SRT temperature increasing with Sm concentration. Magnetic compensation observed in all compositions diminished with Sm doping. We identified Type-I spin switching under specific conditions and compositional ranges. Notably, spin switching depends on the magnitude of the applied magnetic field and the initial temperature during FCC. The sample's magnetic and thermal history plays a significant role in this phenomenon. A magnetic field-T_{SSW} phase diagram, constructed from FCC and FCW data, maps out the magnetic configurations observed.

Invited talk, Fri./17:00

Molecular beam epitaxy: principles, techniques, and advanced applications

E. Piskorska-Hommel[1,2]

[1]*Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Okólna 2, 50-422 Wrocław, Poland*
[2]*Łukasiewicz Research Network - PORT Polish Center for Technology Development, Stabłowicka 147, 54-066 Wrocław, Poland*

email: `e.piskorska@intibs.pl`

Molecular Beam Epitaxy (MBE) is a sophisticated epitaxial growth technique widely recognized for its capability to precisely engineer thin films at an atomic level. It operates under conditions significantly deviating from thermodynamic equilibrium, demanding ultra-high vacuum (UHV) environments [1, 2]. This unique operational characteristic allows for the production of ternary and quaternary compounds with concentrations exceeding those achievable in equilibrium conditions.

The growth principle in MBE is primarily reliant on the kinetic processes involved in atom or molecule beam interactions with substrates maintained at elevated temperatures. This carefully controlled interaction facilitates the precise alignment of the deposited atoms with the substrate lattice, resulting in highly ordered epitaxial films. Consequently, MBE is extensively employed in the synthesis of advanced semiconductor materials owing to its exceptional control over composition and crystal structure.

Reflection high-energy electron diffraction (RHEED) is commonly employed to monitor surface structure and layer growth dynamics. Additionally, post-growth, in situ characterization methods offer comprehensive insights into the epitaxial layers' physical and chemical properties immediately following deposition. Techniques such as X-ray photoelectron spectroscopy (XPS) and Auger electron spectroscopy provide detailed information about the chemical composition and surface states, while scanning electron microscopy (SEM) and atomic force microscopy (AFM) reveal morphological and topographical features at nanoscale resolutions. The epitaxial layers need also more complementary and sophisticated methods to study the crystal quality, electrical, optical and magnetic properties such as X-ray Diffraction, Photoluminescence (PL), and synchrotron techniques: X-ray Absorption Spectroscopy (XAS).

In conclusion, molecular beam epitaxy's unparalleled precision, coupled with sophisticated in situ and ex situ analytical methodologies, establishes it as a critical technique in advanced semiconductor research and technology development. This comprehensive approach enables researchers to prepare and investigate complex semiconductor materials, ultimately facilitating innovations across electronics, optoelectronics, and spintronics.

[1] M. Herman and H. Sitter, Molecular Beam Epitaxy, Springer Verlag, 1996
[2] B. A. Joyce and T. B. Joyce, J. Cryst. Growth, 264 (2004), 605-619

Invited talk, Fri./17:30

Studying magnetic nanomaterials using neutron scattering

A. Glavic

PSI Center for Neutron and Muon Sciences, 5232 Villigen PSI, Switzerland

email: `artur.glavic@psi.ch`

Neutrons are well established as probe to investigate various aspects of condensed matter. With the nuclear and magnetic dipole interactions, 1u mass as well as high penetration power scattering of neutrons is well suited to study structure, magnetism and dynamics on the Å to µm range. I will give an overview on techniques used in the study of nanoscale materials from 5 to 100 nm with some example applications. Depending on the sample geometry and scientific applications the use of small angle neutron scattering (SANS), reflectometry (NR) or grazing incidence scattering (GISANS) give inside into magnetic structures and their correlations. One recent example is the study of frustrated artificial spin structures using GISANS [1] as illustrated in Figure 1.

A large consortium of countries, including Poland, are currently building the European Spallation Source (ESS) that hosts 15 modern neutron beamlines [2]. With this landmark facility, Europe positions itself in a leading position in neutron-based science. These modern instruments will provide outstanding performance that surpasses existing facilities by one to two orders of magnitude, allowing completely new science to be done. As with the existing European facilities, ESS will have an open user program to perform neutron experiments from any scientist, providing successful proposals. I will give a quick overview over the instrument suite with some details on the available SANS instruments as well as the novel small-sample polarized reflectometer Estia, which is based on the focusing reflectometry concept [3] to allow small samples down to 1x1mm^2 to be investigated.

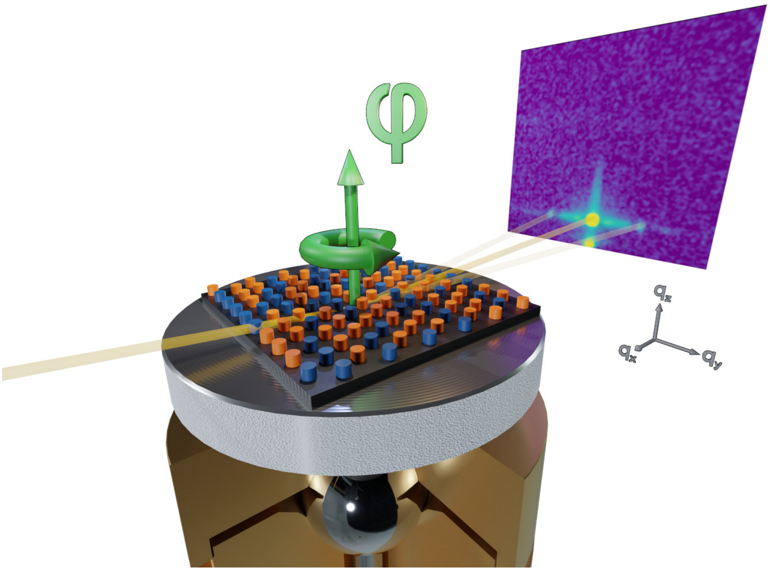

Figure 1: Sketch of neutron scattering under grazing incidence

[1] P. Pip *et al.*, Nanoscale Horiz., 6 (2021), 474-481
[2] K. H. Andersen *et al.*, Nuc. Inst. Meth. A, 957 (2020), 163402
[3] J. Stahn and A. Glavic, Nuc. Inst. Meth. A, 821 (2016), 44-54

Contributed talk, Fri./18:00

Topological in-gap chiral edge states in superconducting Haldane model with spin-orbit coupling

S. Sekh and A. Ptok

Institute of Nuclear Physics Polish Academy of Sciences, PL-31342 Krakow, Poland

email: `sajid.sekh@ifj.edu.pl`

Topological superconductivity is currently one of the prime interests given the properties of its exotic nature of chiral edge states. A broken time-reversal symmetry (TRS) is an essential ingredient in the recipe of a chiral edge state. Haldane model is one of the many factors that can break TRS in a system. Thus, we explore the possibility of topological superconductivity in the Haldane model under the influence of a conventional superconductor. The edge states originating from such recipes mostly remain outside the superconducting gap. Contrary to this, in the presence of spin-orbit coupling, the edge modes lie within the superconducting gap, and can lead to a gapless state for some range of parameters. Moreover, we use band-inversion, and projection on the real-space lattice to confirm the topological and chiral nature of the obtained edge states.

POSTER SESSION

Poster No. 1

Structural diversity and the impact of guest molecules on magnetic properties of CN-bridged coordination polymers

M. Heczko and M. Fitta

Institute of Nuclear Physics Polish Academy of Sciences, Kraków, Poland

email: `michal.heczko@ifj.edu.pl`

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

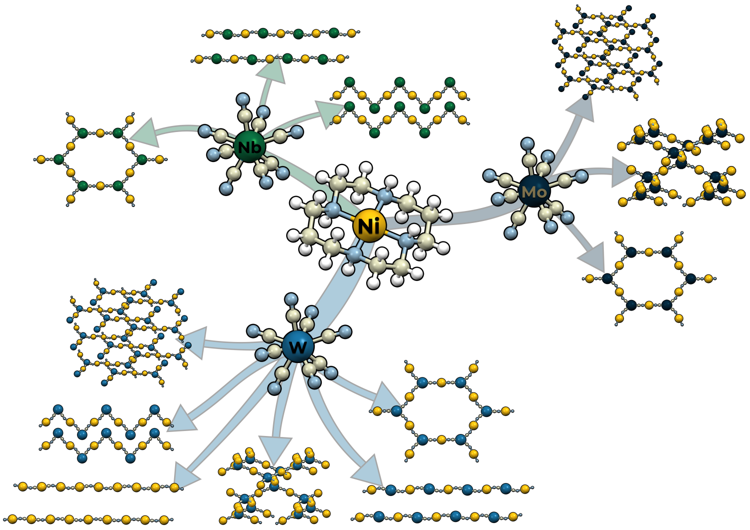

Figure 1: The scheme of reaction pathways leading to coordination networks characterized by different dimensionalities and topologies [1–3]

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

POSTER NO. 2

Comprehensive analysis of the electronic structure of Cu nanoparticles under controlled oxidizing environments

G. Imbir[1], A. Wach[2], J. Czapla-Masztafiak[1], W. Błachucki[1], and J. Szlachetko[2]

[1]*Institute of Nuclear Physics Polish Academy of Sciences, Radzikowskiego 152, 31-342 Krakow, Poland*
[2]*SOLARIS National Synchrotron Radiation Centre, Czerwone Maki 98, 30-392 Krakow, Poland*

email: `gabriela.imbir@ifj.edu.pl`

Nanoparticles (NPs) composed of transition metals such as Au, Ag, and Cu exhibit strong optical responses due to the excitation of localized surface plasmons (LSPs)—collective oscillations of conduction electrons induced by light. These resonances enable unique light-matter interactions, making such nanostructures promising for optical and catalytic applications. Copper, in particular, has emerged as a cost-effective alternative to noble metals [1]. However, Cu NPs are highly susceptible to oxidation, especially below 50 nm [2]. Oxidation occurs rapidly under ambient conditions, necessitating the use of protective core-shell structures to preserve their properties. While encapsulation inhibits oxidation, it also alters the NPs' optical and electronic behavior, hindering systematic studies of their fundamental characteristics.

This study addresses these challenges through comprehensive physicochemical analysis of Cu NPs exposed to oxidation. Using X-ray absorption spectroscopy (XAS), we focus on probing the electronic surface states in CuO_x@Cu core-shell structures. Measurements on two distinct NP sizes enabled separation of bulk and surface contributions affected by oxidation. The results show that the Cu/Cu-oxide composition can be reliably characterized via XAS (Fig.1). Furthermore, oxidation can be effectively tuned by adjusting the concentration of oxidizing agents, such as through the addition of excess H_2O_2. These findings provide a basis for determining Cu/Cu-oxide compositions and deconvoluting their respective contributions

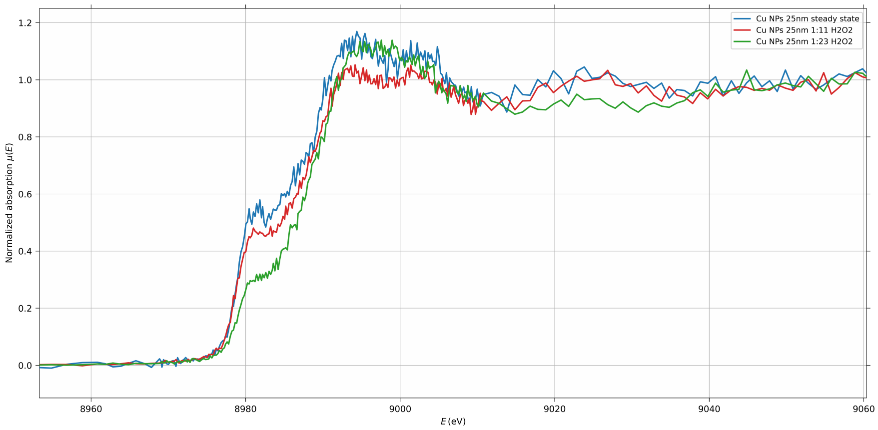

Figure 1: Changes in Cu NPs 25 nm upon oxidation with H_2O_2, tracked by XAS.

Acknowledgements: The authors would like to acknowledge National Science Centre, Poland (NCN) for support under grant no. 2020/37/B/ST3/00555.

[1] S. Mubeen *et al.*, Nat. Nanotechnol., 8 (2013), 247
[2] V.G. Kravets *et al.*, Chem. Rev., 118 (2018), 5912

Poster No. 3

Preparation of a porous coordination polymer for electrochemical ion insertion

J. Karpiel[1], B. Nowicka[1], A. Pacanowska[2], and M. Fitta[2]

[1] *Jagiellonian University, Faculty of Chemistry, Gronostajowa 2, Kraków, Poland*
[2] *Institute of Nuclear Physics Polish Academy of Sciences, Radzikowskiego 152, Kraków, Poland*

email: `julia.karpiel@student.uj.edu.pl`

In hexacyanocobaltate(III), the Co^{3+} ion is located in an octahedral environment of strong-field cyanide ligands, which results in a very stable LS d^6 ($t_{2g}{}^6 e_g{}^0$) configuration. Therefore, in contrast to its hexacyanoferrate(III) analogue, the reduction of Co(III) to Co(II) with LS d^7 ($t_{2g}{}^6 e_g{}^1$) configuration remains a significant challenge yet to be achieved. We aim to attempt reduction of the $[\mathrm{Co}^{III}(\mathrm{CN})_6]^{3-}$ ion in a bimetallic coordination polymer via electroreduction process with guest cation insertion. For this purpose we synthesized $[\mathrm{Ni(cyclam)}]_3[\mathrm{Co(CN)_6}]_2\cdot 15\mathrm{H_2O}$ (cyclam = 1,4,8,11-tetraazacyclotetradecan) in the reaction of $[\mathrm{Ni(cyclam)(NO_3)_2}]$ with $\mathrm{K_3[Co(CN)_6]}$ by two methods - quick precipitation and slow diffusion in an H-tube. The compound shows microporous 2D structure of honeycomb topology (Figure 1). The channels that run across the layers are filled with crystallisation water and can potentially accommodate guest cations. The compound is characterised by reversible water vapor sorption, which occurs gradually, with the formation of several transitional phases differing in the number of water molecules and crystal structure, as shown by powder X-ray diffraction studies.

To prepare the compound for electrochemical ion insertion, thin films were deposited on different conductive substrates using three methods: drop-casting, dip-coating, and sequential growth. The drop-casted films were obtained on PET-ITO foil, gold-sputtered foil and copper plates from nanocrystallites suspension. The films show good surface coverage and thickness of a few micrometres. Films obtained by sequential growth on gold-sputtered foil are thin (∼100 nm) and continuous (Figure 1).

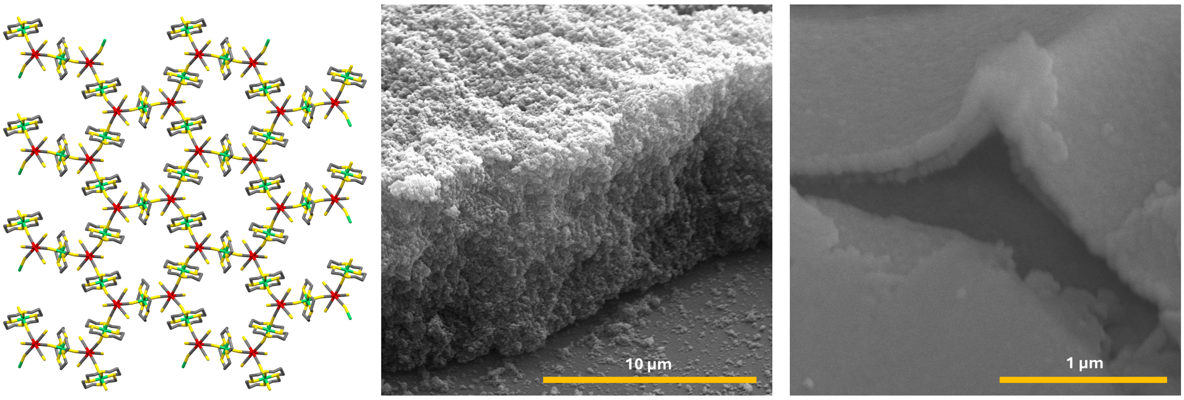

Figure 1: Fragment of structure of $[\mathrm{Ni(cyclam)}]_3[\mathrm{Co(CN)_6}]_2\cdot 15\mathrm{H_2O}$ (left) and SEM images of films obtained by drop-casting (middle) and sequential growth method (right).

Poster No. 4

Isomers of Iron (III) oxides and Cobalt (III) oxides and their redox properties. Quantum-chemical insights.

L. Komando and M. Bobrowski

Gdansk University of Technology, Narutowicza 11/12, 80-233 Gdańsk, Poland

email: `leonard.komando@pg.edu.pl`

Iron (III) oxide and cobalt (III) oxide can form distinct spatial and spin configurations. The kite, spindle and linear molecular clusters have all revealed to be stable for the given spins. The smallest energy state of the Iron (III) oxide cluster is the nonet (S=4) kite configuration and the high-spin states (spin=5) for the spindle and linear structures. In case of cobalt (III) oxide, the linear structure has the lowest energy state, and its electronic configuration is the nonet, as it is revealed from the MP2 computations. Both reduction or oxidation reactions change the geometry and spin of the systems, sometimes transforming one isomer into another. Iron trioxides exhibit standard reduction potentials calculated against the SHE spanning from -3.52 V to -0.43 V, depending particularly on the geometry of the oxide and the method employed. In the case of cobalt trioxides, the standard reduction potentials span from -0.70 V to 1.35 V. The ionization potential ranges from about 7 eV to 10 eV for iron oxides and from about 9 eV to more then 10 eV for cobalt oxides. The electron affinity ranges from about -1 eV to about 4 eV for iron oxides and from 0 eV to about 3 eV for cobalt oxides. The values, however, greatly depend on the method employed and variant of the isomer. Hence, it is revealed that the iron (III) and cobalt (III) oxides are about three times more vulnerable to undergoing one-electron reduction than oxidation. The kite Fe_2O_3 and linear Co_2O_3 are the most vulnerable to reduction. Analogically, the kite configuration of an iron oxide and the linear molecule of a cobalt oxide are the least susceptible to being oxidized because they manifest the largest ionization potentials. Both the iron (III) and cobalt (III) oxides should be considered as relatively good redox agents.

Poster No. 5

Phonon chiral edge modes in EuPtSi and $NbSi_2$

I. Mahraj and A. Ptok

Institute of Nuclear Physics, Polish Academy of Sciences, W. E. Radzikowskiego 152, PL-31342 Kraków, Poland

email: `mahraj.issam@gmail.com`

An object is considered chiral if it cannot be superimposed onto its mirror image. A chiral system is characterized by a unique crystal structure in which atoms arrange into chiral chains along a specific direction, forming a distinctive chiral framework. In such systems, chiral edge modes can emerge for both electrons and phonons, propagating unidirectionally and connecting two points with opposite topological charges in the first Brillouin zone.

In this study, we investigate EuPtSi and $NbSi_2$, which possess $P2_13$ and $P6_222$ chiral symmetries, respectively, by analyzing their bulk and slab phonon properties using *ab initio* techniques. The bulk phonon band structure of EuPtSi reveals a spin-1 Weyl point at the Γ point and a charge-2 Dirac at R point. Similarly, $NbSi_2$ exhibits two Weyl points at Γ and K point. These topological features in the band structure give arise to the formation of *Fermi arcs*, which connect those with opposite topological charges (*Chern number*). Consequently, the surface states of EuPtSi and $NbSi_2$ exhibit chiral edge modes.

For both compounds, the phonon chiral edge states extend from the center to the edge of the Brillouin zone. However, $NbSi_2$ displays a distinct behavior, with *Fermi arcs* exhibiting momentum-dependent characteristics.

[1] I.Mahraj and A.Ptok, arXiv:2409.12807.

Poster No. 6

Theoretical study of hydrogen binding and hydrogen activation on metal-decorated circumcoronene and borophene nanoflakes

M. Malček and O. Tkáč

Institute of Physical Chemistry and Chemical Physics, Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava, Radlinského 9, SK-812 37 Bratislava, Slovak Republic

email: `michal.malcek@stuba.sk`

An interaction between the hydrogen molecules and two-dimensional or finite-size nanomaterials is nowadays extensively studied, both experimentally and theoretically. The ultimate aim of such studies is to design novel materials capable of storing hydrogen molecules at ambient conditions. In this respect, hydrogen binding and storage performance of circumcoronenes and borophene nanoflakes decorated with various transition metals (TM) is investigated using density functional theory [1, 2]. The studied systems show affinity to bind hydrogen molecules in two distinct ways, i.e. formation of η^2-H_2-bond (Kubas interaction) [3] or dissociation of H_2 molecule leading to H_2 activation. It is found that the systems decorated with light TM atoms, such as Sc or Ti, are more suitable for dissociation of H_2 molecule while the systems decorated with heavier TM atoms, such as Co or Ni preferably bound H_2 molecules via Kubas interactions. These findings are in agreement with earlier reports on the H_2 binding preference of TM-decorated carbon nanotubes [4]. Further insights into the nature of TM-H_2 interaction in these systems are obtained from Bader's quantum theory of atoms in molecules and ab initio molecular dynamics simulations.

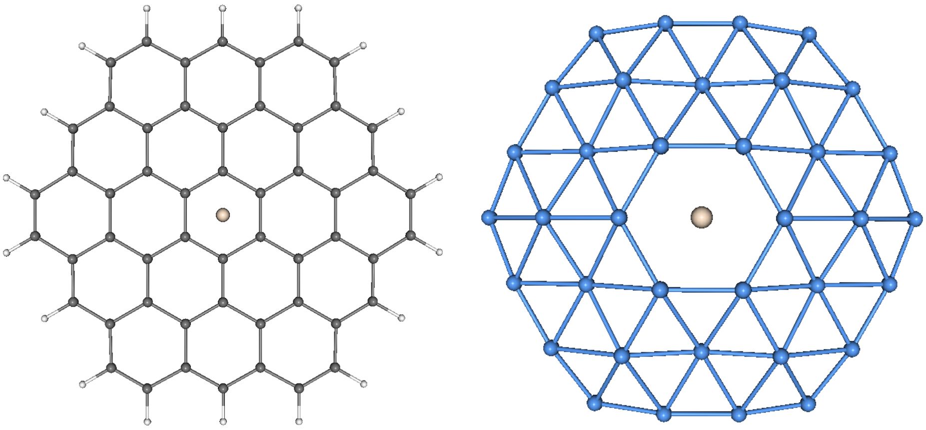

Figure 1: Metal-decorated circumcoronene (left) and borophene nanoflake (right).

Acknowledgements: We are grateful to the Slovak Grant Agencies APVV (contracts No. APVV-20-0213, APVV-23-0006, and VV-MVP-24-0039) and VEGA (contract No. 1/0324/24), and SIVVP project (ITMS code 26230120002) for computational resources.

[1] S. Müllerová *et al.*, Carb. Lett., 34 (2024), 1495-1506
[2] K. Tančárová *et al.*, FlatChem, 49 (2025), 100799
[3] G. J. Kubas, J. Organomet. Chem., 751 (2014), 33-49
[4] H. Valencia *et al.*, J. Phys. Chem. C, 119 (2015), 5506-5522

Poster No. 7

Interfacial charge transfer complexes between TiO_2 and organic molecules - insight from DFT and spectroscopic methods

M. Malček Šimunková[1], V. Lazić[2], D. Sredojević[2], D. Dvoranová[1], and M. Malček[1]

[1] *Institute of Physical Chemistry and Chemical Physics, Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava, Radlinského 9, SK-812 37 Bratislava, Slovak Republic*

[2] *Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, Centre of Excellence for Photoconversion, P.O. Box 522, 11001, Belgrade, Serbia*

email: `miriama.simunkova@stuba.sk`

The "Achilles heel" of photocatalytic materials based on TiO_2 polymorphs is the effective production of reactive oxygen species (ROS) only upon UVA excitation. The activation of TiO_2 by more practical visible light is limited by its wide band gap energy, e.g. anatase, with the band gap $\sim$ 3.2 eV, absorbs less than 5% of the available solar light, which can initiate the formation of photogenerated electron-hole pairs and thus stimulates the redox processes on the catalyst surface [1]. The formation of interfacial charge transfer (ICT) complexes by condensation reaction between wide-bandgap metal oxides and small organic molecules provides a simple way to obtain visible-light-responsive materials. The activation of the ICT complexes by visible (VIS) light is a result of the carefully balanced electronic structure and energetic considerations of the donor-acceptor system, allowing efficient absorption of VIS-light and subsequent charge transfer. Until now, strong ICT transitions have been exclusively reported between surface Ti atoms and aromatic compounds with either two adjacent hydroxyl groups (catecholate-type ligands) or adjacent hydroxyl and carboxyl groups (salicylate-type ligands) [2]. In our study, the TiO_2-based ICT complex with taxifolin, a flavonoid with antioxidant ability, displays light absorption in the visible spectral range. The results obtained using the density functional theory (DFT) calculations on a cluster model were in excellent agreement with spectroscopic measurements. The spin trapping and spin scavenging revealed the differences between the behavior of the pristine and surface-modified TiO_2 powders with taxifolin before and upon excitation. The results provide a solid base for further studies of potential applications of photo-driven processes in oxide-based hybrids activated in the visible spectral range.

Acknowledgements: This study was supported by APVV projects VV-MVP-24-0039, SK-SRB-23-0021 and the call for doctoral students and young researchers of Slovak University of Technology in Bratislava to start a research career (Grant 23-04-02-B).

[1] Z. Barbieriková *et al.*, J. Catal., 331 (2015), 39-48
[2] V. Nikšić *et al.*, Opt. Mater., 152 (2024), 115454

Poster No. 8

Investigation of the effectiveness of selected absorbers in the protection of mammalian cells against the effects of ionizing radiation

N. Mendelska[1,2], A. Trębińska-Stryjewska[1], Ł. Osuchowski[1], A. Sitkiewicz[1], and Z. Mierczyk[1]

[1] *Biomedical Engineering Centre, Institute of Optoelectronics, Military University of Technology, ul. gen. Sylwestra Kaliskiego 2, 00-908 Warsaw, Poland*
[2] *Doctoral School, Military University of Technology, ul. gen. Sylwestra Kaliskiego 2B, 00-908 Warsaw, Poland*

email: `natalia.mendelska@wat.edu.pl`

Ionizing radiation poses a significant threat to living organisms, leading to DNA damage, genetic mutations and the development of neoplastic lesions [1]. To evaluate potential bioprotection strategies, studies were conducted on DU-145 cancer cells, analyzing their viability and metabolic response after exposure. The test subject were absorbers which were tested, including epoxy composites doped with heavy metal nanoparticles, whose protective properties derive from their ability to absorb and attenuate ionizing radiation [2]. Figure 1 shows the effectiveness of various absorbers in lowering the power of the radiation source, which translates into a degree of cell protection. The results indicate varying effectiveness of the materials and mechanisms analyzed, confirming the need for further research into their application in biomedicine and radiation protection.

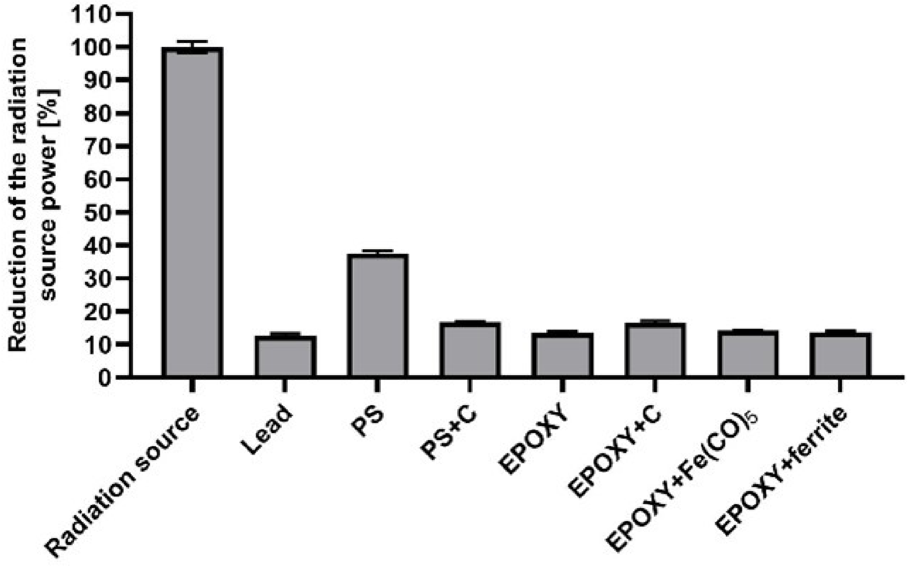

Figure 1: Percentage reduction in ionizing radiation source power for selected absorbers.

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Poster No. 9

Spectral measurements of soft X-ray emission from a laser-produced plasma source based on an aerosol target

W. Rafalak, Ł. Węgrzyński, T. Fok, M. Majszyk, A. Bartnik, and H. Fiedorowicz

Institute of Optoelectronics, Military University of Technology, Kaliskiego 2 00-908 Warsaw, Poland

email: `wiktoria.rafalak@wat.edu.pl`

Soft X-ray radiation with wavelengths in the nanometer range of approximately 1-10 nm can be efficiently generated by focusing nanosecond laser pulses with energy of the order of a single Joule on a gas puff target created by pulsed injection of high-pressure gas into the laser focus region. The use of a gas puff target instead of a solid target avoids the deleterious effects of target debris generated by laser ablation of the solid. Laser-plasma soft X-ray sources based on gas puff target have found application in many fields, including imaging of biological structures with nanometer resolution [1], XAFS spectroscopy of transition metals [2] and optical coherence tomography of nanolayers [3].

A certain limitation of gas puff targets is the small number of gases that can be used to generate plasma, which has an adverse effect on the spectral characteristics of the soft X-ray radiation produced. A solution to this problem may be the use of gas puff targets containing additional material in the form of small micrometer-sized droplets produced from liquids of different elemental composition (aerosol targets). Such targets can be produced by injecting a mist generated by a piezoelectric atomizer into the laser focus [4].

The paper presents the results of studies on the emission of soft X-ray radiation from an aerosol target containing iodine and cesium irradiated with laser pulses of about 1 ns duration and energy up to 5 J. Emission spectra of radiation in the wavelength range from 2 nm to 12 nm have been recorded using a spectrometer with a transmission grating coupled to a CCD camera.

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Poster No. 10

National Synchrotron Radiation Centre SOLARIS: the unique facility in Central and Eastern Europe

A. Toboła-Galus, M. Jaglarz, and D. Raś

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

email: `agata.tobola-galus@uj.edu.pl`

The National Synchrotron Radiation Centre SOLARIS is the first synchrotron in Poland. It is an advanced accelerator device that accelerates electrons to high velocities, close to the speed of light. The change in the direction of accelerated particles in the magnetic field of the synchrotron causes the emission of electromagnetic radiation known as synchrotron radiation. This radiation is extremely intense and has a wide spectrum from infrared to X-rays. Due to their unique properties, synchrotrons are used in many fields of science and technology, including physics, chemistry, biology, materials science, and even archaeology, enabling detailed studies of the structure and properties of matter at the atomic and molecular levels [1].

The facility provides access to infrastructure for hundreds of researchers annually, requiring appropriate safety coordination. This includes daily use of the facility, maintenance work around the accelerator tunnels, and chemical and biological risks associated with materials brought by users.

An important aspect of our operations is ensuring radiological safety in the working environment. Radiation levels are continuously monitored using radiation monitoring stations (RMSs), thermoluminescent dosimeters (TLDs), and radiometers [2]. Additionally, our research infrastructure includes a Personal Safety System (PSS) designed to protect personnel and users from entering areas with high levels of ionizing radiation. In hazardous situations, this system automatically halts the synchrotron operation to ensure safety.

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Poster No. 11

Low-angle X-ray photoelectron spectroscopy in the analysis of gold nanolayers

G. Wesołowski[1], A. Kubala-Kukuś[1,2], D. Banaś[1,2], K. Szary[1,2], I. Stabrawa[1,2], P. Jagodziński[1,3], M. Pajek[1], M. Borysiewicz[4], O. Sadowski[4], and J. Chojenka[5]

[1] *Institute of Physics, Jan Kochanowski University, Uniwersytecka 7, 25-406 Kielce, Poland*
[2] *Holy Cross Cancer Center, Artwińskiego 3, 25-734 Kielce, Poland*
[3] *Central Office of Measures, Elektoralna 2, 00-139 Warsaw, Poland*
[4] *Łukasiewicz Research Network - Institute of Microelectronics and Photonics, al. Lotników 32/46, 02-668 Warsaw, Poland*
[5] *Institute of Nuclear Physics Polish Academy of Sciences, Radzikowskiego 152, 31-342 Kraków, Poland*

email: `s131403@student.ujk.edu.pl`

X-ray photoelectron spectroscopy (XPS) is a powerful technique for surface analysis, and its sensitivity can be significantly enhanced when used in low-angle configuration [1, 2]. In this study, total reflection XPS (TRXPS), were applied to investigate gold nanolayers (10 nm, 50 nm, 100 nm) deposited on silicon substrates. The goal of the research was to determine the suitability of the TRXPS method in terms of its ability to study the elemental composition, surface homogeneity, and to discuss the detection limits achieved by TXRF. The TRXPS measurements were conducted at a low incidence angle (2.4°), being below critical angle for primary beam energy 1486 eV (Al-Kα) and Au material, and enabling improved surface sensitivity. The experiments were conducted at the Institute of Physics, Jan Kochanowski University in Kielce, Poland.

Results demonstrate that TRXPS provides surface sensitivity better than standard XPS and can detect low-concentration elements with an improved limit of detection. In TRXPS geometry, the detection limit improves by a factor of 2-7 depending on incidence angle and element analyzed.

For studied Au nanolayer, grazing incidence X-ray photoelectron spectroscopy (GIXPS) [3] curves where also calculated to evaluate the angular dependence of the photoelectron yields in regime of low angles. GIXPS calculations enable modeling of depth-sensitive photoelectron yields and reveals that gold layers thicker than 5 nm exhibit similar angular response, indicating bulk-like type of sample. Therefore this method shows potential for characterizing nanolayers below 5 nm in thickness.

The combination of experimental XPS/TRXPS results with theoretical GIXPS modeling offers a complementary framework for quantitative and depth-sensitive analysis of ultrathin metallic nanolayers. The presented results will support future research on nanostructure formation induced by highly charged ion beams.

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