Zakopane School of Physics



Breaking Frontiers: Submicron Structures in Physics and Biology

 $23-27\ \mathrm{May}\ 2023$



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PROGRAM OF THE CONFERENCE

TUESDAY, 23 MAY 2023

16:00	REGISTRATION

- 18:00 **Dinner**
- 18:50 **Opening of the Conference**
 - **Opening lecture Wojciech Tabiś** (Kraków, Poland)
- 19:00 Exploring High Magnetic Field Facilities: Advancements, Challenges, and Appli- p.8 cations

WEDNESDAY, 24 MAY 2023

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9:00	Probing ultrafast structural and electronic dynamics in chemistry, biology and materials research using X-ray free electron lasers	p. 11
9:30	Katarzyna Jarzembska (Warszawa, Poland) Tracing of transient species in small-molecule crystals using photocrystallographic techniques	p. 12
9:50	Rafał Fanselow (Kraków, Poland) Clocking ultrashort processes in matter with X-ray Chronoscopy	p. 13
10:05	Anna Niedźwiecka (Warszawa, Poland) Intrinsically disordered proteins that regulate fundamental biological processes – challenging targets for biophysical studies	p. 14
10:20	Jerzy Antonowicz (Warszawa, Poland) Structural pathways for ultrafast melting of optically excited thin polycrystalline palladium films	p. 15
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11:30	Cristian Svetina (Madrid, Spain) Extension of four wave-mixing methods at short wavelengths	p. 18
12:00	Tomasz Fok (Warszawa, Poland) Compact NEXAFS system based on a laser-plasma soft X-ray light source	p. 19
12:15	Mateusz Gala (Kraków, Poland) Role of intrinsic and external strain on the Verwey phase transition in magnetite	p. 20
12:30	Naveen Singh Dhami (Zagreb, Croatia) Hydrostatic pressure effects on electronic and crystal structures of non- centrosymmetric $EuTGe_3$ ($T = Co$, Rh, and Ir)	p. 21

12:45	Mohammad Sadegh Shakeri (Kraków, Poland) How pulsed laser irradiation of suspended nanoparticles utilizes for production of Cu-CuO-Cu ₂ O heterostructure as catalyst for energy applications	p. 22		
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17:00	Jakub Szlachetko (Kraków, Poland) SOLARIS National Synchrotron Radiation Centre: the infrastructure for research and industry Gabriela Imbir (Kraków, Poland)	p. 31		
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15 00	Bohdan Padlyak (Zielona Góra, Poland)	
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16:45	Bringing molecular photomagnets to light – photochemical approach to molecular photomagnets	p. 67
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17:30	Pavlo Baloh (Košice, Slovakia) Experimental study of magnetic properties of Dv(PO ₃) ₃ glass	p. 69
	Dominik Czernia (Kraków, Poland)	
17:45	The unconventional methods of tailoring magnetic properties in molecular mag- nets: proton and plasma treatments	p. 70
18:00	Closing remarks	
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7:00	BREAKFAST	

DEPARTURE TO KRAKÓW

8:30

Opening lecture, Tue./19:00

Exploring High Magnetic Field Facilities: Advancements, Challenges, and Applications

<u>W. Tabiś^{1,2}</u>

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High magnetic field facilities are an essential tool for research in various areas, including condensed matter physics and materials science. The presentation will provide an overview of high magnetic field facilities, with a focus on resistive and pulsed magnet technologies that can generate fields up to megagauss strength.

The talk will cover the capabilities of high magnetic field facilities for studying the properties of materials under extreme conditions, including the electronic and magnetic properties of magnetic materials. Examples of research will be presented, highlighting the applications of high magnetic field facilities in the study of novel materials and the potential for these facilities to enable new types of experiments and scientific discovery.

Technological advances that have enabled the development of high magnetic field facilities, such as advances in pulsed power technology, will be shortly discussed. The limitations and challenges of high magnetic field facilities will also be addressed, along with future directions and potential breakthroughs in this field.

Overall, this presentation will provide a comprehensive overview of the capabilities and potential of high magnetic field facilities in the study of magnetic and superconducting materials, and highlight the exciting research opportunities that are opening up in this rapidly developing field.

Acknowledgements: We acknowledge the support from NCN (grant OPUS: UMO-2021/41/B/ST3/03454), and NAWA ('Polish Returns 2019' Program: PPN/PPO/2019/1/00014).

SESSION I: RESEARCH PROSPECTS AT XFEL

Chair: Jakub Szlachetko

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	Katarzyna Jarzembska (Warszawa, Poland)	
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0.50	Rafał Fanselow (Kraków, Poland)	n 13
3.00	Clocking ultrashort processes in matter with X-ray Chronoscopy	p. 15
	Anna Niedźwiecka (Warszawa, Poland)	
10:05	Intrinsically disordered proteins that regulate fundamental biolog-	p. 14
	ical processes – challenging targets for biophysical studies	
	Jerzy Antonowicz (Warszawa, Poland)	
10:20	Structural pathways for ultrafast melting of optically excited thin	p. 15
	polycrystalline palladium films	

Invaited talk, Wed./8:30

Multi-photon processes and molecular dynamics in the soft X-ray regime: The Small Quantum Systems (SQS) instrument at the European XFEL

M. Meyer

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The Small Quantum Systems (SQS) scientific instrument at the European X-ray Free Electron Laser in Germany is dedicated to investigations on atoms, molecules, clusters and nanoparticles. The instrument is installed behind the SASE3 soft X-ray undulator, which produces intense X-ray pulses in the photon energy range between 250 eV and 3000 eV. The accelerator is generally delivering up to 3500 pulses per second to the SQS instrument with pulse energies of up to 10 mJ. These characteristics in combination with pulse durations in the range of 10 to 30 fs provide an ideal basis for numerous investigations involving site-selective core excitations with a special focus on non-linear phenomena and the dynamics of ultrafast processes.

First scientific investigations were concentrating on multi-photon processes using high-resolution electron, ion and electron-ion coincidence spectroscopy as well as on studies of larger systems using coherent diffraction imaging (e.g. [1–3]). The experiments covered processes of (resonant) multiple ionization, above threshold ionization (ATI), double core hole (DCH) formation and stimulated X-ray Raman scattering (SXRS) in atoms as well as X-ray induced dissociation dynamics of small molecules monitored via Coulomb explosion imaging (CEI), and highlighted the excellent performances of the instrument. In the talk, after the presentation of the SQS instrument, some examples of current scientific results as well as future applications in the attosecond time domain will be discussed.

- [1] G. Kastirke et al., Phys. Rev. X, 10 (2020) 021052
- [2] U. Eichmann et al., Science, 369 (2020) 1630
- [3] T. Mazza et al., Phys. Rev. X, 10 (2020) 041056

Invaited talk, Wed./9:00

Probing ultrafast structural and electronic dynamics in chemistry, biology and materials research using X-ray free electron lasers

C. J. Milne

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X-ray spectroscopy and scattering allow a unique combination of electronic and structural information to be obtained from a variety of different types of samples in many different forms (solid, liquid, gas). The extension of these methods into the time domain has allowed measurement of dynamic processes, for example the tracking the photoinduced charge carriers in a functional material [1] or following the photocycle in a light activated protein [2]. In recent years X-rays have started to become routinely used to measure light-activated processes using a pump-probe scheme, where the sample is photoexcited with light and then probed after a variable time delay using an X-ray pulse. These methods can measure dynamics over a broad range of timescales, allowing them to probe everything from protein dynamics to ultrafast electronic spin-state changes in molecular systems. With the recent development of X-ray free electron lasers (XFELs), time-resolved X-ray techniques have moved into the ultrafast regime, where the timescales of electron and nuclear motion can be accessed using the femtosecond X-ray pulses available from these facilities.



Figure 1: Layout of the FXE instrument for ultrafast X-ray measurements with some typical X-ray measurements displayed

This talk will present an overview of how X-ray techniques are being used at XFELs and the type of information the measurements can provide. The talk will introduce the European XFEL, a brandnew, high-repetition rate XFEL facility located in northern Germany, and its' Femtosecond X-ray Experiments (FXE) instrument [3] which is focussed on measuring ultrafast dynamics in the condensed phase. Finally the lecture will present some examples of the types of measurements XFELs can perform and the scientific questions that can be answered using ultrafast X-ray techniques.

- T. J. Penfold *et al.*, Nat. Comm., 9 (2018) 478; M. H. Rittmann-Frank *et al.*, Angew. Chem. Int. Ed., 53 (2014) 5858-5862
- [2] C. Bacellar et al., P. Natl. Acad. Sci. Usa., 117 (2020) 21914-21920; D. Kinschel et al., Nat. Comm., 11 (2020) 4145
- [3] D. Khakhulin et al., Appl. Sci., 10 (2020) 995; A. Galler et al., J. Syn. Rad., 26 (2019) 1-16.

Contributed talk, Wed./9:30

Tracing of transient species in small-molecule crystals using^{Zakopane} photocrystallographic techniques

K. Jarzembska , R. Kamiński , and P. Łaski

Department of Chemistry, University of Warsaw, Warszawa, Poland

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Whereas studies of light-induced effects in solutions are rather well-developed nowadays, the solidstate investigations of this kind are much more demanding, thus less established. Nevertheless, solidstate materials applications are of great and constantly increasing significance, ranging from sensors, optoelectronic devices and ultra-high capacity data storage media, to environmental and biomedical applications. Therefore, a considerable volume of effort should be dedicated to studies of materials in their technologically-applicable solid-state form. In this respect, single crystals are unique due to well-defined three-dimensional structure. This property makes them excellent model systems to mimic real-world situations, but also to supplement the solution-sample studies, or model the intersurface environment. Since light-induced processes cause structural distortions (new bond formations, atom oxidation state changes, etc.), in the case of crystals they can be explored via X-ray diffraction techniques.

Hence, in this contribution we will present current possibilities of time-resolved photocrystallography for small-molecule crystals. The results of our latest synchrotron studies dedicated to photoactive transition-metal complexes in the solid state will serve as examples [1, 2]. Additionally, we will discuss research perspectives emerging once XFEL radiation is applied.



Figure 1: Photodifference map for dicarbonyl (4-bromo-N-salicylideneaniline)rhodium(I). Blue isosurfaces represent influx of electron density of at least $0.35 \text{ e}\cdot \text{A}^{-3}$.

Acknowledgements: SONATA BIS (2020/38/E/ST4/00400), NSC (Poland), Support for Polish Eu-XFEL users–Supervision, Part II (2022-26), Ministry of Science and Education (Poland), South African National Research Foundation (137759), Advanced Photon Source, BioCARS beamline (R24GM111072) NIH (U.S.). Development of TR setup at BioCARS possible via collaboration with Philip Anfinrud (NIH/NIDDK).

- [1] K. N. Jarzembska *et al.*, Crystals, 9 (2019) 36
- [2] K. N. Jarzembska et al., Inorg. Chem., 53 (2014) 10594-10601

Contributed talk, Wed./9:50

Clocking ultrashort processes in matter with X-ray Chronoscopy^{ane}

<u>R. Fanselow¹</u>, W. Błachucki¹, and J. Szlachetko²

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The development of X-ray Free Electron Lasers (XFELs) unlocked new possibilities in many areas of science. These facilities produce femtosecond X-ray pulses with extremely high peak brilliance, providing an unmatched tool to study ultrashort phenomena in matter. However, some fundamental electron processes, for instance, the initial stages of charge carriers relaxation in semiconductor systems, are too fast to be spectroscopically traced even with the shortest available XFEL pulses. Recently, we proposed an innovative methodology called X-ray Chronoscopy to bypass current time resolution limits at XFELs facilities [1]. The method focuses on measuring changes in time profiles of the incident and transmitted X-ray pulse induced by interaction with a sample. Such an experiment could be realized with the implementation of well-established terahertz streaking techniques. In the present study, we show that the X-ray Chronoscopy method can be applied to time-dependent pump-probe experiments at femtosecond time scales to follow charge dynamics in zinc selenide semiconductor nanocrystals induced by ultrashort optical pulses (Fig. 1). By applying simple four-state atomic model, we investigated how X-ray probe pulse duration influences the measurement of the material excited state relaxation rates.



Figure 1: a) Scheme of an optical pump – X-ray probe experiment; b) calculated temporal profiles of pump and probe pulses.

Acknowledgements: This project was financed by National Science Centre (Poland) under grant number 2017/27/B/ST2/01890

[1] W. Błachucki et al., Appl, Sci., 12 (2022) 1721

Contributed talk, Wed./10:05

Intrinsically disordered proteins that regulate fundamental biological processes – challenging targets for biophysical studies

<u>A. Niedźwiecka¹</u>, M. K. Cieplak-Rotowska^{1,2,3}, M. K. Białobrzewski², and B. Klepka²

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Intrinsically disordered proteins (IDPs) with their dynamic structure often serve in nature as a kind of molecular switches that regulate fundamental processes in living organisms. Their structural dynamics is directly related to their biological function. The key role here is played by the partial or complete lack of a fixed spatial structure, allowing flexible adaptation to interacting protein partners, RNA or ligands. Such proteins and interaction within their complexes are not amenable to structural studies by traditional methods such as X-ray crystallography or multidimensional nuclear magnetic resonance due to the significant proportion of structurally disordered fragments, large molecular sizes or limited solubility. Studies of the properties and interactions of such biopolymers at the molecular level require alternative physical and biophysical methods, such as, for example, proton-deuterium exchange coupled with mass spectrometry [1] or fluorescence correlation spectroscopy. We will present our recent results obtained for two classes of intrinsically disordered proteins: the human GW182 protein involved in gene silencing [2] and the AGARP protein regulating the process of biomineralization in the skeletal organic matrix of Acropora millepora corals [3]. Learning about the characteristics of these proteins brings us closer to understanding the physical bases of the most important biochemical processes on which the proper development and functioning of eukaryotic organisms depends, and to explaining fundamental issues related to the history of life on Earth – the mass appearance of skeletons of organisms, e.g. corals.

Acknowledgements: The work was supported by the NCN grant no. UMO-2016/22/E/NZ1/00656.

- [1] M.K. Cieplak-Rotowska et al., J Am Soc Mass Spectrom, 29 (2018) 158-173
- [2] M.R. Fabian *et al.*, Nat Struct Mol Biol, 18 (2011) 1211-1217
- [3]P. Ramos-Silva $et\ al.,$ Mol Biol Evol, 30 (2013) 2099-2112

Contributed talk, Wed./10:20

Structural pathways for ultrafast melting of optically excited thin polycrystalline palladium films

<u>J. Antonowicz</u>¹, A. Olczak¹, K. Sokolowski-Tinten², P. Zalden³, I. Milov⁴, P. Dzięgielewski¹, and R. Sobierajski⁵

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²Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany
³European XFEL, Schenefeld, Germany
⁴Industrial Focus Group XUV Optics, MESA+ Institute for Nanotechnology, University of Twente, NB Enschede, Netherlands
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Due to its extremely short timescale, the non-equilibrium melting of metals is exceptionally difficult to probe experimentally. The knowledge of melting mechanisms is thus, to a large extent, based on the results of theoretical predictions and computer modeling. This work reports on the ultrafast melting of thin polycrystalline Pd films studied by an optical laser pump – X-ray free-electron laser probe technique [1] and two-temperature model molecular dynamics simulations. By acquiring the X-ray diffraction snapshots with a picosecond resolution, we capture the sample's atomic structure during its transition from the crystalline to the liquid state. Bridging the timescales of the experiment and the simulation allows us to formulate a comprehensive microscopic picture of the melting transition. We demonstrate that the melting process gradually accelerates with the increasing density of the absorbed energy. The molecular dynamics simulations reveal that the transition mechanism progressively varies from heterogeneous, initiated inside structurally disordered grain boundaries, to homogenous, proceeding catastrophically in the crystal volume on a picosecond timescale close to that of electron-phonon coupling in Pd [2].



Figure 1: False-color representation of diffraction patterns plotted as a function of the optical pump – X-ray probe delay time (a) and absorbed energy density (b).

[1] P. Zalden *et al.*, Science, 364 (2019) 1062-1067

[2] N. Medvedev et al., Phys. Rev. B, 102 (2020) 064302

SESSION II: APPLICATIONS OF MODERN X-RAY TECHNIQUES

Chair: Chris Milne

	Przemysław Piekarz (Kraków, Poland)	
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11:50	Extension of four wave-mixing methods at short wavelengths	
	Tomasz Fok (Warszawa, Poland)	
12:00	Compact NEXAFS system based on a laser-plasma soft X-ray light	p. 19
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	Mateusz Gala (Kraków, Poland)	
12:15	Role of intrinsic and external strain on the Verwey phase transition	p. 20
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	Naveen Singh Dhami (Zagreb, Croatia)	
12:30	Hydrostatic pressure effects on electronic and crystal structures of	p. 21
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	Mohammad Sadegh Shakeri (Kraków, Poland)	
12:45	How pulsed laser irradiation of suspended nanoparticles utilizes for	p 22
	production of Cu-CuO-Cu ₂ O heterostructure as catalyst for energy	r
	applications	

INVAITED TALK, WED./11:00

Theoretical study of the demagnetization process in magnetic^{kopane} multilayers under ultrafast X-ray irradiation

<u>P. Piekarz</u>¹, K. J. Kapcia^{2,3}, V. Tkachenko^{2,4}, F. Capotondi⁵, A. Lichtenstein^{4,6}, S. Molodtsov⁴, L. Müller⁷, A. Philippi-Kobs⁷, and B. Ziaja^{1,2}

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We investigated the X-ray induced ultrafast demagnetization of magnetic multilayer systems using the newly developed modeling tool called XSPIN. It enables to simulate the electronic processes in X-ray irradiated ferromagnetic materials. We studied the specific response of the Co/Pt multilayer system irradiated by an ultrafast XUV pulse at the *M*-edge of Co (photon energy about 60 eV). The results were compared with the experimental data obtained at the FERMI free-electron-laser facility, using the magnetic small-angle X-ray scattering technique (mSAXS). The simulations show that the magnetic scattering signal from Co decreases on the femtosecond timescales due to electronic excitation, relaxation and transport processes both in the Co and Pt layers [1]. The signal decrease scales with the increasing fluence of incoming radiation, following the trend observed in the experimental data. A similar theoretical study was performed for the Co/Pd multilayers irradiated by X-ray pulses tuned to the *L*-edge of Co (photon energy about 778 eV). We found that, like in the case of X-ray-induced demagnetization at the *M*-edge of Co, electronic processes play a main role in the demagnetization until the pulse fluence does not exceed the structural damage threshold [2]. Confirmation of the predominant role of electronic processes for X-ray induced demagnetization is a step towards quantitative control and manipulation of X-ray induced magnetic processes on femtosecond timescales.

- [1] K. J. Kapcia et al., npj Comput. Mater., 8 (2022) 212
- [2] K. J. Kapcia et al., Phys. Rev. B, 107 (2023) 094402

Invaited talk, Wed./11:30

Extension of four wave-mixing methods at short wavelengths^{akopane}

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Four wave-mixing optical domain techniques represent a major advance in experimental and theoretical physics, chemistry, Atomic-Molecular and Optical (AMO) physics as well as in biology. The nonlinear response of a sample under the influence of multiple laser beams allows to measure fundamental properties such as electronic response, propagation of wave-packets, electron-phonon coupling, phonons, transport phenomena and magnetic properties of the sample. Transient Grating (TG) is a four wave-mixing method employing two crossed laser beams interacting at the sample to generate an interference pattern and a third time-delayed probe beam to monitor the time evolution of the induced dynamics that transiently changes the index of refraction. TG is widely used in the optical domain to gain information on transport and diffusion processes as well as on charge-magnetic and vibrational dynamics. Extension of TG, and more generally wave-mixing, at short wavelengths would open the possibility to ultimately reach (sub)-nanometer and (sub)-femtosecond scales adding element and chemical specificity having direct access to K, L and M shells. In the first half of the talk I will give a brief introduction of nonlinear optics and describe the TG method and its features in the optical regime and its extension in the Extreme Ultraviolet range at FERMI Free Electron Laser (FEL) [1]. In the second half I will dive into the extension of TG in the X-rays applying the Talbot effect [2] (Fig.1), showing experimental results at X-ray FELs [3] and discuss about the many possible evolutions of the methodology.



Figure 1: Artistic representation of X-ray Transient Grating generated via Talbot effect and probed with a third time delayed pulse.

- [1] F. Bencivenga et al., Nature, 520 (2015) 205-208
- [2] C. Svetina et al., Opt. Lett., 44 (2019) 574-577
- [3] J. R. Rouxel et al., Nat. Photon., 15 (2021) 499-503

Compact NEXAFS system based on a laser-plasma soft X-ray light source

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Near-edge X-ray absorption fine structure (NEXAFS) spectroscopy is one of the most important metrology methods available in synchrotrons facility. To enable such research in smaller laboratories just a few groups design compact devices with lower, but still useful energy ranges.

One of the solutions is a system designed and tested in the Laser Matter Group at the Military University of Technology. This compact NEXAFS system is based on a laser plasma source where a dual stream gas puff target is irradiated by nanosecond Nd:YAG laser. Depending on the gas target we obtained an efficient emission in the photon energy range of 200-600 eV (Kr/He) [1] or above 700 eV up to 1 keV (Xe/He) [2]. That energy range gives access to investigate low-Z material near the K-edge, e.g. C, N, O, or havier elements near the L-edge such as Fe, Co, Ni [3]. This unique measuring system allows registering of the reference and sample spectra at the same time. The system enables transmission mode measurement of thin samples up to several hundred nanometers thick, which can be deposited on SEM grids or SiN membranes. The measurement setup and NEXAFS measurement results using this compact measurement setup will be presented.

Acknowledgements: The research was supported by European Union's Horizon 2020 Programme (LASERLAB-EUROPE) Grant Agreement No. 871124 and the university research grant UGB No. 23/IOE/2022.

- [1] T. Fok et al., J. Phys. Chem. Solids, 164 (2022) 110623
- [2] P. Wachulak et al., Opt. Express, 29 (2021) 120514
- [3] T. Fok et al., Materials 14, (2021) 7337

Contributed talk, Wed./12:15

Role of intrinsic and external strain on the Verwey phase transition in magnetite

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Magnetite belongs to one of the most extensively studied magnetic materials for its functional applications, e.g., in medicine or IT. Around $T_V \approx 123$ K, it exhibits a semimetal to insulator phase transition, called the Verwey transition (VT) [1], which is still not completely understood [2]. VT is associated with the change of the crystallographic structure from cubic (above T_V) to monoclinic, and with the modification of the electronic properties, which are reflected, e.g., in electrical resistivity $\rho(T)$ which changes by 2 orders of magnitude on crossing T_V . Although all the processes that are responsible for VT are still not known, magnetic interactions leading to ferrimagnetism may be of high importance [3]. Also, electronic inhomogeneities, distributed across the material either local (nm) or global (μ m) scale may play a role in VT. These inhomogeneities may be static or dynamic and their evolution (and thus triggering the transition itself) may be affected by application of stress. We investigated the influence of the intrinsic and externally induced strain on the electronic phase separation in single crystals of Fe₃O₄. Maps of mosaicity and internal strains were collected using Dark Field X-ray Microscopy at ID06, ESRF. We also measured $\rho(T)$ as a function of uniaxial pressure applied along [100] up to 500 MPa and observed a systematic increase of T_V with pressure.

Acknowledgements: We acknowledge the support from NCN (grant OPUS: UMO-2021/41/B/ST3/03454), and NAWA ('Polish Returns 2019' Program: PPN/PPO/2019/1/00014).

- [1] E.J. Verwey et al., Physica, 8 (1941) 979
- [2] W. Wang et al., arXiv:2202.08744v3, (2022)
- $[3]\,$ G. Perversiet
al., Nat. Comm., 10 (2019) 2857

Contributed talk, Wed./12:30

Hydrostatic pressure effects on electronic and crystal structures of non-centrosymmetric $\text{Eu}T\text{Ge}_3$ (T = Co, Rh, and Ir)

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Intermetallic EuTX₃ (T: transition metal, X = Si/Ge) forms a non-centrosymmetric BaNiSn₃-type structure (space group I4mm). It has been attracting considerable attention due to complex magnetic structures and unique pressure phase diagram that potentially accommodates superconductivity under pressure [1]. At ambient pressure, all EuTGe₃ series host divalent Eu ions $(4f^7, J = 7/2)$ and exhibit antiferromagnetic ordering at low temperatures (<15 K). In order to study the T-dependent pressure behavior of the electronic and crystal structures of $EuTGe_3$ (T = Co, Rh, Ir), we performed high energy resolution fluorescence detected X-ray absorption spectroscopy (XAS) and powder X-ray diffraction (XRD) as a function of pressure at the GALAXIES and PSICHE beamlines of SOLEIL Synchrotron. In all compounds, a prominent Eu^{2+} peak was observed in the Eu L_3 XAS spectra at ambient pressure. With increasing pressure, these spectra revealed a continuous change towards an intermediate Eu valence state. The mean Eu valence reached ≈ 2.4 near 40 GPa [2] in EuRhGe₃, and ≈ 2.5 and ≈ 2.3 near 50 GPa in EuIrGe₃ and EuCoGe-3 [3], respectively. In the latter compound, the Ge K and Co K edge XAS spectra showed no remarkable changes against pressure [3]. The results of high-pressure powder XRD exhibited a smooth contraction of the lattice volume without any symmetry changes in EuRhGe₃ and EuCoGe₃. While the result of EuIrGe₃ indicated a pressure-induced structural transition around 34 GPa. Our study revealed the pressure evolution of Eu valence and crystal structure of EuTGe₃. Details of the differences in pressure response of Eu valence and crystal structure arising from different nature among 3d, 4d and 5d transition metal ions will be discussed in the oral presentation.

Acknowledgements: The work is supported by the Croatian Science Foundation project numbers UIP-2019-04-2154 and IP-2020-02-9666.

- [1] M. Nakashima et al., J. Phys. Soc. Jpn., 86 (2017) 034708
- [2] Y. Utsumi et al., Electron. Struct., 3 (2021) 034002
- [3] N. S. Dhami *et al.*, accepted to Phys. Rev. B.

Contributed talk, Wed./12:45

How pulsed laser irradiation of suspended nanoparticles utilizes for production of Cu-CuO-Cu₂O heterostructure as catalyst for energy applications

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Laser-matter interaction has fascinated the scientific community with its enormous novel applicability. More specified when it comes to the laser-suspension interaction, it is still frontier but promising for a bunch of partially studied applications e.g. synthesis, and also its prospect in separation, particle coding, microscopy, and so on due to the temperature selectivity authorized by the functionality of absorption-size. The phase formation resulting from pulsed laser irradiation of suspended nanoparticles has recently been introduced as a high-potential synthesizing technique for heterostructures. The main challenge still lingers regarding the exact particle formation mechanism due to non-equilibrium kinetical byproducts resulting from the local alternative ultra-fast high-temperature nature of the process. Here, we analyze the bond breaking/formation of distinct copper and cupric interfaces with ethanol during absorption of laser pulses for the possible formation of Cu-CuO-Cu₂O heterostructure applicable as an electrocatalyst for ethanol oxidation fuel cell and photo-catalyst for water splitting $(H_2 \text{ evolution as green energy})$. Exploiting absorption rules, the temperature of agglomerates was calculated followed by the introduction of a particle growth mathematical model. We showed that the local interface of dissociated ethanol and the melted sphere is responsible for the divergent diffusion of oxygen and carbon compounds engaging in the oxidation/reduction processes thanks to the reactive bond force field molecular dynamics studies confirmed by ab-initio calculations and experimental observations. Resulted composite powder also showed remarkable catalysis behavior mostly applicable as the renewable energy material.

Acknowledgements: This work is supported by the Polish National Science Centre Programs No. 2018/31/B/ST8/03043 and 2022/06/X/ST3/01743. The computational parts were executed in Cyfronet, Krakow using Grant No. PLG/2022/015573.

- [1] M. S. Shakeri et al., Sci. Rep., 12:1 (2022) 1-15
- [2] H. Wang et al., J/ Amer. Chem. Soc., 133:47 (2011) 19102-19109.
- [3] A. Kowal et al., Nat. Mat., 8:4 (2009) 325-330.1

SESSION III: MOLECULAR MAGNETISM

Chair: Mark Meisel

Beata Nowicka (Kraków, Poland)	
Thin films and nanocomposites of switchable coordination poly-	p. 24
mers	
Alicia Forment-Aliaga (Valéncia, Spain)	n 25
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Piotr Konieczny (Kraków, Poland)	
The versatility of low dimensional molecular magnets on examples	p. 26
of magnetocaloric effect	
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Luminescent molecular nanomagnets based on lanthanide(III)	p. 27
complexes and octacyanidometallates(IV)	
Petro Danylchenko (Košice, Slovakia)	
Preparation, characterization and magnetic properties of	n 98
$Cu(en)(H_2O)_2SO_4$ inserted in a hexagonal self-ordered meso-	p. 20
porous silica SBA-15	
	 Beata Nowicka (Kraków, Poland) Thin films and nanocomposites of switchable coordination polymers Alicia Forment-Aliaga (Valéncia, Spain) Spin-crossover effect meets 2D materials and chirality Piotr Konieczny (Kraków, Poland) The versatility of low dimensional molecular magnets on examples of magnetocaloric effect Robert Jankowski (Kraków, Poland) Luminescent molecular nanomagnets based on lanthanide(III) complexes and octacyanidometallates(IV) Petro Danylchenko (Košice, Slovakia) Preparation, characterization and magnetic properties of Cu(en)(H₂O)₂SO₄ inserted in a hexagonal self-ordered mesoporous silica SBA-15

Invaited talk, Wed./14:00

2023

Thin films and nanocomposites of switchable coordination polymers

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Molecule-based magnetic materials are usually obtained in the form of crystals, which are characterized by unfavorable mechanical properties. Surface deposition or dispersion in an organic polymer matrix of is an important step towards exploration of the application potential of these compounds. The aim of our work was the preparation of thin films and nanocomposites of CN-bridged networks, which show switchability of magnetic properties in response to changes of temperature, pressure, or humidity[1, 2]. We employed different physical and chemical methods of film fabrication, depending on the formation processes and stability conditions of the networks. They included the bottom-up approach of in situ formation of the coordination network on the substrate surface as well as the top-down approach of crystal size reduction by ultrasonic and mechanical homogenization or modification of synthetic conditions. We investigated how different deposition techniques influence the film morphology and how the switchable properties of the bulk samples are affected by the grain size reduction and interface interactions (Figure 1) [3]. We have also prepared nanocomposites consisting of coordination network particles embedded in the organic polymer matrix in the form of surface deposited membranes or electrospun mats.



Figure 1: Morphology and magnetism of the $\{[Ni(cyclam)]_3[Cr(CN)_6]2 \cdot nH_2O\}_n$ thin films.

- [1] B. Nowicka et al., Cryst Growth Des., 16 (2016) 4736
- [2] M. Reczyński et al., Angew. Chem. Int. Ed., 60(2021) 2330
- [3] A. Pacanowska et al., Adv. Mater. Interfaces, 10 (2023) 2201834

Zakopane

Invaited talk, Thu./14:30

Spin-crossover effect meets 2D materials and chirality

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Among magnetic molecular materials, spin crossover (SCO) compounds are specially interesting due to their behavior as molecular switches. Therefore, their magnetic, electronic, optical, and structural properties can be modulated by external stimuli like temperature, light or pressure. These coordination compounds are mainly based on Fe (II) and can be nanostructured as nanoparticles without losing their properties [1].

In this presentation I would like to show how SCO compounds can work as molecular tools to modulate the electronic and optical properties of two-dimensional materials (2D), giving rise to smart 2D heterostructures where the optoelectronic properties of the 2D layers are reversibly modulated by strain induced through switchable SCO nanoparticles, Fig. 2a [2].



Figure 1: a) Transmission electron microscopy image of MoS_2 2D layers functionalized with SCO nanoparticles with a schematic representation of the system. b) Crystalline structure of Λ -RR enantiomer of an iron based chiral SCO compound and a summary of optical (top) and magnetic (bottom) properties of both enantiomers.

On the second part of my talk (Fig. 1b), we will explore the possibility of combining SCO and chirality looking for (1) the design of novel multifunctional magneto-optical materials and (2) the role that the spin of the metallic ion can play in the spin filtering properties of chiral molecules (the intriguing Chiral Induce Spin Selectivity, CISS, effect) [3].

- [1] J. A. Real et al., Dalton Trans., 12 (2005) 2062-2079
- [2] R. Torres-Cavanillas et al., Nat. Chem., 13 (2021) 1101-1109
- [3] R. Torres-Cavanillas et al., J. Am. Chem. Soc., 142:41 (2020) 17572-17580

Contributed talk, Wed./15:15

The versatility of low dimensional molecular magnets on examples of magnetocaloric effect

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Modern coordination chemistry provides a wide scope of functional molecular magnet platforms revealing different coordination dimensionality, from the discrete molecules (0D) through the chain (1D) and layered (2D) sub-structures towards the fully extended (3D) systems. Apart from the fundamental role of local atomic/molecular features of interest (size, symmetry, electron transfer, chirality, electronic properties, etc.), which are important for the desired properties, in many cases, the target functionality emerges by their coordination dimensionality. One of the crucial modern applications of low-dimensional molecule magnets is the magnetocaloric effect.

The magnetocaloric effect (MCE) refers to the temperature change in a magnetic material upon application or removal of a magnetic field. Research has shown that low-dimensional molecular magnets exhibit strong MCE due to their unique magnetic properties and enhanced magnetic interactions. The study of MCE in these materials has important implications for the development of energy-efficient cooling technologies. This research aims to explore the MCE in various low-dimensional molecular magnets and to understand the underlying physical mechanisms that contribute to the effect.



Figure 1: The idea of rotating magnetocaloric effect.

- [1] P. Konieczny et al., Inorg. Chem., 56 (2017) 2777-2783
- [2] P. Konieczny et al., Sci. Rep., 12 (2022) 16601
- [3] P. Konieczny et al., Dalton Trans., 51 (2022) 12762-80

2023

Contributed talk, Wed./15:30

Luminescent molecular nanomagnets based on lanthanide (III)^{opane} complexes and octacyanidometallates (IV)

<u>R. Jankowski</u>¹, J. J. Zakrzewski¹, M. Zychowicz¹, J. Wang², Y. Oki², D. Pinkowicz¹, B. Sieklucka¹, and S. Chorazy¹

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Lanthanide(III) single-molecule magnets (Ln^{III} -SMMs) constitute a rich source of multifunctionality since they connect the field of luminophores, applicable in i.a. light-emitting diodes, with an area of molecular nanomagnets, a potential key to high-density data storage devices, offering other advantages, e.g., magneto-optical correlations and emission adjustable by a magnetic field [1]. In the pursuit of multifunctional molecular nanomagnets, we explored the group of bimetallic $Ln^{III}-[M^{IV}(CN)_8]^{4-}$ assemblies [2, 3]. Here, we show a few examples of Ln^{III} -SMMs based on anionic Mo(IV) and W(IV) octacyanidometallates and selected NIR emissive lanthanide(III) complexes, uncovering the modulating role of these metalloligands in the sensitization and tuning of the 4*f*-metal-centred emission and their impact on magnetic relaxation processes. Potential possibilities for further functionalization of such cyanido-bridged assemblies will also be discussed.



Figure 1: Magnetic and optical features of selected $\text{Ln}^{\text{III}}[M^{\text{IV}}(\text{CN})_8]^{4-}$ assemblies: temperaturedependence of magnetic relaxation times for $\{[\text{Nd}_{111}^{\text{III}}(\text{H}_2\text{O})_17(\text{pzdo})_5][M^{\text{IV}}(\text{CN})_8]_3\}$ (pzdo= pyrazine N,N'-dioxide; M = Mo (red), W (blue); left) and NIR emission spectra for (PPN)[Yb^{\text{III}}(\text{pzdo})_2(\text{MeOH})_{0.3}(\text{H}_2\text{O})_{3.7}][M^{\text{IV}}(\text{CN})_8] (M = Mo (blue), W (purple); right).

- [1] R. Marin et al., Angew. Chem. Int. Ed., 60 (2021) 1728-1746
- [2] R. Jankowski et al., J. Mater. Chem. C, 9 (2021) 10705-10717
- [3] R. Jankowski et al., Inorg. Chem. Front., 6 (2019) 2423-2434

Contributed talk, Wed./15:45

Preparation, characterization and magnetic properties of $Cu(en)(H_2O)_2SO_4$ inserted in a hexagonal self-ordered mesoporous silica SBA-15

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The main aim of our work is to successfully synthesize $Cu(en)(H_2O)_2SO_4$ (en – ethylenediamine) complex into the pores of mesoporous silica SBA-15 to attain new stable hybrid material, with highest possible degree of pore filling. Therefore we carry out the synthesis process with the free parameter of the time which the silica being in saturated solution of $Cu(en)(H_2O)_2SO_4$. The chosen times of synthesis are 90 minutes, 24 hours, 72 hours and 14 days. The amount of complex presented in the hybrid material is equal up to 160 mmol on each 100 g of hybrid material, for the samples with synthesis time more than 24 hours. The EPR study shows that emergence of new peaks on $Cu(en)(H_2O)_2SO_4@SBA15$ sample compare to the $Cu(en)(H_2O)_2SO_4$ could be interpreted by the distortion of crystallographic structure and manifestation of the hyperfine interaction of Cu(II) nuclei. For the hybrid sample the obtained value of f-factor (g_z/A_z ratio) is 221.77 cm⁻¹, which is reasonable near to the typical value 250 cm^{-1} for tetrahedral complexes. Temperature dependence of magnetic susceptibility for complex $Cu(en)(H_2O)_2SO_4$ inside the pores SBA-15 arise continuously with increasing temperature and shows paramagnetic behavior without any phase transition to magnetically ordered state in contradistinction to the bulk $Cu(en)(H_2O)_2SO_4$ complex, where it has been observed at $T_N=0.91 \text{ K}$ [1].

Acknowledgements: This work was supported by the Slovak Research and Development Agency Project number APVV-18-0197 and VEGA Grant No. 1/0132/22 of the Scientific Grant Agency of the Ministry of Education, Science, Research and Sport of the Slovak Republic.

[1] M. Kajňaková et al., Phys. Rev. B 71, (2005) 014435

SESSION IV: APPLICATIONS OF MODERN X-RAY TECHNIQUES

Chair: Cristian Svetina

16:30	Claudio Cirelli (Villigen, Switzerland) Ultrafast X-ray science at SwissFEL Alvra	p. 30
17:00	Jakub Szlachetko (Kraków, Poland) SOLARIS National Synchrotron Radiation Centre: the infrastruc- ture for research and industry	p. 31
17:30	Gabriela Imbir (Kraków, Poland) Characterization of plasmonic nanostructures based on pH- dependent gold nanoparticles using X-ray Absorption Spectroscopy	p. 32
17:45	Wojciech Błachucki (Kraków, Poland) Coupling two timing tools at SwissFEL	p. 33
18:00	Wiktoria Stańczyk (Kraków, Poland) BioXAS examination of copper-phenanthroline complexes in solu- tions with biomolecules	p. 34

Zakopane

Invaited talk, Wed. /16:30

Ultrafast X-ray science at SwissFEL Alvra

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Over the last decade, X-ray free electron lasers (XFELs) have emerged as one of the most powerful tools to understand physical and chemical properties of matter and investigate ultrafast processes on the pico- to femtosecond timescale. This new class of light sources are able to produce ultrashort, intense bursts of X-ray radiation that are ideally suited to perform ultrafast spectroscopy and imaging experiments in the XUV, soft and hard X-ray photon energy range.

The Aramis hard X-ray beamline of the Swiss X-ray free electron laser SwissFEL started regular user operation in January 2019. Since then, it has been continuously increasing its performance with respect to lasing and timing stability, pulse energy and repetition rate, allowing for the successful realization of many novel experiments.

The Alvra instrument at SwissFEL is focused on the investigation of ultrafast photochemical and photo-biological processes, offering a range of X-ray techniques, including serial femtosecond crystallography (SFX), X-ray solution scattering (XSS), and X-ray absorption and emission spectroscopy (XAS and XES).

In my talk, I will review the capabilities and developments of the Alvra endstation and I will discuss our recent efforts to implement multimodal experiments using multiple techniques simultaneously over the full Aramis photon energy range of 2-12.4 keV.

The capability of performing ultrafast spectroscopy in the tender X-ray (2-5 keV) with high signalto-noise and temporal resolution makes the Alvra endstation unique and particularly appealing for the local and international XFEL user community. Invaited talk, Wed./17:00

SOLARIS National Synchrotron Radiation Centre: the infrastructure for research and industry

J. Szlachetko

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The SOLARIS [1] synchrotron in Krakow is a third-generation synchrotron radiation source operating in the medium electron energy range. The first synchrotron light in SOLARIS was observed in 2016, while the first user experiments were performed in 2018. SOLARIS is expanding its activities, constantly developing experimental beamlines and complementary infrastructure such as cryoelectron microscopes. Research opportunities offered by SOLARIS, the only synchrotron in Central and Eastern Europe, allow for conducting unique scientific projects in fundamental research and applied sciences. It should be emphasized that access to the research infrastructure in SOLARIS is free of charge and provided based on the assessment of the beamtime applications by the international review panel. In the presentation, we will present the SOLARIS synchrotron project and available infrastructure, provide practical information on access to the infrastructure, and show examples of the research results obtained at the Centre by the Users.

[1] J. Szlachetko et al., Eur. Phys. J. Plus, 138 (2023) 10

Contributed talk, Wed./17:30

Characterization of plasmonic nanostructures based on pH-dependent gold nanoparticles using X-ray Absorption Spectroscopy

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As nanostructure materials, gold nanoparticles (Au NPs) stand out by high chemical stability, surface functionalization, but most of all, unique optical properties induced by localized surface plasmon resonance (LSPR). It was reported that surface environment of Au NPs is responsible for tuning LSPR, which is highly desirable for biomedical applications [1]. Zhang *et al.*found that the presence of *d* electrons on the surface is related to capping agent selection, i.e., stabilizers that prevent from uncontrolled NPs growth [2]. Others showed that LSPR indicated strong dependence on Au NPs shape [3]. However, there is still much unknown about influence of LSPR to electronic and chemical behavior of Au NPs.

In presented studies, citrate-stabilized gold nanoparticles were subjected to different chemical environments by modifying pH of capping agent and examine for physical and chemical properties. Au NPs were analyzed using spectroscopic techniques, mainly X-ray Absorption Spectroscopy (XAS) and visible light (UV-VIS). The surface morphology was visualized using Transmission Electron Microscopy.

Based on preliminary XAS experiments, presented on Figure 1, difference in spectra, both in XANES and EXAFS area (maximize chart), was found between each analyzed nanoparticles type. The obtained results within this work will help to correlate the pH-dependence of Au NPs with LSPR shifting and to closely study the surface physicochemical features.



Figure 1: X-ray absorption spectra of different types of Au NPs obtained by inverse Turkevich method obtained at Swiss Light Source facility

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

- [1] J. M. Ramallo-López et al., Phys. Rev. B, 74 (2006) 073410
- [2] P. Zhang *et al.*, J. Chem. Phys., 81 (2002) 184701
- [3] H. Bin Jeon *et al.*, Scien. Rep., 9 (2019) 13635

Zakopane

Contributed talk, Wed./17:45

Coupling two timing tools at SwissFEL

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Several direct measurement methods are employed at X-ray free-electron lasers (XFELs) in pulse arrival time measurement: spectral encoding [1], spatial encoding [2] and THz streaking [3]. In this work, the THz streaking and the spatial encoding timing tools available at SwissFEL in Paul Scherrer Institute (Villigen, Switzerland) were coupled in series and the precision of arrival time measurement was studied for 300 µJ pulses of 7230 eV photons. The distributions of arrival time and arrival time difference obtained for 6140 pulses are presented in Fig. 1. As shown, the coupling of two timing tools has improved the timing precision two times. The coupling of individual timing tools can considerably improve the resolution of time-resolved pump-probe experiments.



Figure 1: Arrival times measured with methods: THz streaking (t_{THz}) and spatial encoding (t_{Spatial}) .

Acknowledgements: This project was financed by the Swiss National Science Foundation (SNSF) (numbers 1263236, 0968895, 1102301) and The 863 Program (number 2013AA014402). W.B. and J.Sz. acknowledge the financial support of the National Science Centre (Poland) under grant number 2017/27/B/ST2/01890.

- [1] M. R. Bionta et al., Opt. Express, 19 (2011) 21855
- [2] T. Katayama et al., Struct. Dyn., 3 (2016) 034301
- [3] P. N. Juranić et al., J. Instrumentation, 9 (2014) P03006

Contributed talk, Wed./18:00

BioXAS examination of copper-phenanthroline complexes in akopane solutions with biomolecules

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Due to side effects that are observed in anticancer therapy with platinum-based compounds, researchers took into consideration other metals, especially commonly known micronutrients, like iron or copper, in a form of hybrid complexes or nanoparticles [1]. The first studied artificial nuclease was a copper-phenanthroline complex, and from that time it seems that this kind of compound is still very promising for application in medicine.

In the presented research, two copper-phenanthroline complexes were examined with the use of X-ray Absorption Spectroscopy: Cu(1,10-phenanthroline) Cl_2 and Cu(1,10-phenanthroline, 1,2,4-triazole) Cl_2 . The latter complex was synthesized in the chemical laboratory, based on the procedure described in [2]. Two types of X-rays source were used: a synchrotron source DESY, Hamburg, Germany, and an X-ray tube in the Institute of Nuclear Physics PAN, Kraków, Poland [3]. The performed examination was focused on samples in the solid state form, dissolved in water, and in the form of an aqueous solution with added biomolecules (DNA or BSA).

A comparison of the data gathered in both facilities for referential compounds and complexes of interest will be presented. The process of investigation of any possible interactions of complexes with chosen biomolecules will be also discussed.



Figure 1: Comparison of XAS spectra of samples with copper-phenanthroline-triazole complex.

Acknowledgements: The authors would like to acknowledge National Science Centre, Poland (NCN) for support under grant no. 2020/37/B/ST3/00555 and 2016/21/D/ST4/00378.

^[1] P. Szymański et al., Biometals, 25 (2012) 1089-1112

^[2] S. Tabassum et al., Eur. J. Med. Chem., 58 (2012) 308-316

^[3] W. Stańczyk et al., NIMB, 497 (2021) 65-69

SESSION V: NEW IDEAS: MATERIALS AND EXPERIMENTS

Chair: Siham Benhabib

	Ioanna Mantouvalou (Berlin, Germany)	
14:30	Transient NEXAFS spectroscopy using a laser-produced plasma	p. 36
	soft X-ray source	
15.00	Denys Makarov (Dresden, Germany)	- 97
13:00	Curvilinear magnetism: from fundamentals to applications	р. эт
15.20	Bohdan Padlyak (Zielona Góra, Poland)	90
19:90	EPR spectroscopy of the radiation-induced centres in borate glasses	р. зо
16:00	TECHNOLUTIONS	

Invaited talk, Thu./14:30

Transient NEXAFS spectroscopy using a laser-produced plasma soft X-ray source

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Laboratory-based laser-produced plasma (lpp) soft X-ray sources achieve high brightness and stability in the EUV and XUV range. With emission energies beyond 1.6 keV and stable operating times in the range of hours, they offer already numerous experimental possibilities independent and supplemental to investigations at large scale facilities.

One such application is near edge X-ray absorption fine structure (NEXAFS) spectroscopy for the elucidation of the electronic structure of a given sample. In combination with optical pumping also photo-induced dynamics can be probed which shed light on the structure-function relationship of complex materials.

We present a setup for optical pump – soft X-ray probe NEXAFS spectroscopy composed of a highly brilliant lpp source [1] and a reflection zone plate spectrometer [2]. The system can probe X-ray absorption edges between 200 eV and 1400 eV with a resolving power ≈ 1000 . The pump beamline offers a time resolution of 500 ps with a tunable wavelength (343 nm – 900 nm) [3]. Due to the high stability and efficiency of the setup, dynamic changes in absorption of the excited sample down to 10^{-4} are accessible. Application measurements on thin solid and liquid films will be presented demonstrating the capabilities of lab-based instrumentation.

[1] I. Mantouvalou et al., Rev. Sci. Instr., 86 (2015) 035116

- [2] A. Jonas et al., Opt. Express, 27 (2019) 36524-36537
- [3] H. Stiel et al., Int. J. Mol. Sci., 22:24 (2021) 13463
Invaited talk, Thu./15:00

Curvilinear magnetism: from fundamentals to applications Zakopane

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The behaviour of any physical system is determined by the order parameter whose distribution is governed by the geometry of the physical space of the object, in particular its dimensionality and curvature. In magnetism, the coupling between geometry (topology) of a ferromagnet and magnetic order parameter brings about novel responses of curved thin films and nanowires [1]. In thin film limit, local curvatures can force a geometry-driven local interactions like Dzyaloshinskii–Moriya interaction (DMI) and anisotropy as well as novel non-local chiral effects. In addition to activities on geometrically curved ferromagnets, there are recent appealing developments for curvilinear antiferromagnets where curvature effects results in the appearance of chiral responses, helimagnetic phase transitions, weak ferromagnetism and hybridisation of spin wave modes. Contrary to planar non-collinear structures, curvilinear design enables 3D architectures, which can revolutionize magnetic devices with respect to size, functionality and speed. At present, 3D-shaped magnetic architectures are explored as spin-wave filters, racetrack memory, artificial magnetoelectric materials, and shapeable magnetoelectronics for human-machine interfaces and soft robotics [2]. These fundamental and application-oriented topics will be covered in the presentation [3].

- [1] D. Makarov et al., Adv. Mater. (Review), 34 (2022) 2101758
- [2] G. S. Canon Bermudez et al., Adv. Funct. Mater. (Review), 31 (2021) 2007788
- [3] D. Makarov and D. Sheka (Editors), Curvilinear micromagnetism: from fundamentals to applications (Springer, Zurich, 2022). https://link.springer.com/book/10.1007/978-3-031-09086-8

Invaited talk, Thu./15:30

EPR spectroscopy of the radiation-induced centres in borate glasses

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The X-band electron paramagnetic resonance (EPR) spectra of borate glasses with chemical compositions of LiB₃O₅, SrB₄O₇, CaB₄O₇, Li₂B₄O₇, KLiB₄O₇, SrB₆O₁O, and LiCsB₆O₁O, irradiated at room temperature by high doses of γ -rays (10⁷ Gy) and X-rays (1–2·10⁴ R) were registered and interpreted. The undoped borate glasses of high chemical purity and optical quality were obtained from corresponding polycrystalline compounds by fast cooling of their melts according to technological conditions, described in [1]. The EPR spectroscopy of the γ - and X-irradiated borate glasses shows presence radiation-induced paramagnetic centres stable at room temperature practically in all investigated glasses. Detailed analysis of the observed EPR spectra shows that the registered spectra belong to radiation-induced paramagnetic centres that can be described in the framework of model of the O^- hole centres, located in different network sites of the studied glasses. The 4-component EPR spectrum of the O^- centres are related to superhyperfine (SHF) structure, caused by interaction of the unpaired electron spin with one nearest nucleus of the ¹¹B magnetic isotope (nuclear spin I = 3/2, natural abundance -80.1%). In the irradiated borate glasses also were observed weak EPR signal with the 7-component SHF structure that belongs to the O^- centres, localized near one nucleus of the ${}^{10}B$ isotopes (nuclear spin I = 3, natural abundance – 19.9%). Unstructured anisotropic EPR signal, observed in the irradiated borate glasses, is ascribed to the O⁻ hole centres, located in the glass network near non-magnetic isotopes. Observed in the irradiated borate glasses unstructured anisotropic EPR signal was ascribed to the O^- hole centres, located in the glass network near non-magnetic isotopes. EPR spectra of anisotropic O^- hole centres without SHF structure were observed previously by us in the neutron-irradiated $Li_2B_4O_7$ single crystals [2] as well as in the γ - and X-irradiated glasses of the CaO-Ga₂O₃–GeO₂ system [3]. The features of EPR spectra, electronic and local structure of the radiation-induced centres in the borate glasses with different chemical composition are discussed in comparison with available published data of EPR spectroscopy of the γ -, X-, and neutron-irradiated borate crystals and glasses. Possible applications of the studied borate glasses for radiation protection dosimetry as well as for different devices in space systems are considered.

Acknowledgements: This work was supported by scientific project No. 0122U001833 of the Ministry of Education and Science of Ukraine.

- [1] B. V. Padlyak et al., Mater. Sci. Pol. 30 (2012) 264-273
- [2] Ya. V. Burak et al., Nucl. Instr. Meth. Phys. Res. B, 191 (2002) 633-637
- [3] B. V. Padlyak, Radiat. Eff. Defects Solids, 158 (2003) 411-418

SESSION VI: NOVEL MAGNETIC MATERIALS

Chair: Denis Makarov

Session VI: Novel magnetic materials

19:00	Karolina Podgórska (Kraków, Poland) Verwey transition and magnetic correlations in magnetite	p. 40
19:15	Paweł Sobieszczyk (Kraków, Poland) Surface effects in Tb ₂₅ Fe ₇₅ nanoparticles	p. 41
19:30	Juliusz Chojenka (Kraków, Poland) Controlling the photoactivity of nanopatterned titanium oxide	p. 42
19:45	Oliwia Polit (Kraków, Poland) Magnetic properties of copper-iron based composite particles syn- thesized by laser melting in liquid	p. 43
20:00	Brahim Bahloul (M'sila, Algeria) Study of the structural, electronic, magnetic properties of MnCo ₂ Al Compound	p. 44

Contributed talk, Thu./19:00

Verwey transition and magnetic correlations in magnetite Zakopane

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Magnetite, one of the magnetic materials longest known to mankind, is characterised by the spectacular metal-insulator transition (known as Verwey transition) observed around 125 K. Despite intensive research, this transition has not been fully explained. Most of the research conducted on magnetite has focused on its low-temperature phase. In recent years, however, it has been suggested that hightemperature phenomena reaching as high as the Curie temperature (around 850 K) may affect the low-temperature Verwey transition [1, 2].

To better understand the phenomena occurring in the high-temperature phase of magnetite, hightemperature resistivity, magnetisation and AC susceptibility measurements were performed. The studies were carried out on stoichiometric magnetite and 13 samples of $\text{Fe}_{3-x}M_x\text{O}_4$, where (M = Zn, Ti,Al, Mn) with different levels of doping and therefore different T_V . The results of the measurements allowed to determine four characteristic temperatures, i.e. two characteristic temperatures on the resistivity curve $(T_{\text{R1}}, T_{\text{R2}})$, the Verwey temperature (T_V) and the Curie temperature (T_C) .

Analysis of the Curie temperature dependence on the Verwey temperature showed that the two temperatures are scaling with each other with a proportional relationship. This suggests that the magnetic transition and the Verwey transition are correlated, and thus the localization of charges at the Verwey transition may have its origin already at elevated temperatures. In addition, our analysis of the two characteristic temperatures in the resistivity curves shows that although resistivity is sensitive to the magnetic transition, it is not the quantity that should be used to determine the Curie temperature.

Acknowledgements: We acknowledge the support from NCN (grant OPUS: 2021/41/B/ST3/03454, SONATA BIS: 2018/30/E/ST3/00377), and NAWA ('Polish Returns 2019' Program: PPN/PPO/2019/1/00014).

- [1] G. Perversi et al., Nat. Commun., 10 (2019) 2857
- [2] H. Elnaggar et al., Phys. Rev. Lett., 127 (2021) 18

Zakopane

Contributed talk, Thu./19:15

Surface effects in $Tb_{25}Fe_{75}$ nanoparticles

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The great interest of the 3d-transition metal – rare earth ferrimagnetic alloys has been emerged due to their possible applications in magneto-optical recording and ultrafast laser switching [1]. The most interesting properties for the magnetic reorientation process occurs at the compensation temperature (T_n) where no magnetisation appears below Curie temperature. The value of the compensation point can be controlled through the composition and structure of the alloy as well as by ion irradiation and annealing [2]. With the help of Vampire atomistic simulation software [3] we explore other possibilities of tuning the compensation point by changing the bulk to surface ratio. We studied the Tb₂₅Fe₇₅ nanospheres with diameters (D) ranging from 3 nm to 12 nm and it has been observed that T_n depends on the diameter as 1/D, which may be attributed to changes in the spin direction on the nanoparticle surface. We demonstrate how the reduction of the average number of surface neighbors, preferential oxidation, and chemical segregation can change compensation and Curie temperatures as well as magnetic reversal characteristics of the alloy. The results indicate that the preferential oxidation plays a leading role, whereas reduction of average number of neighbors and chemical segregation are found as the second most important factors.



Figure 1: Compensation temperatures determined for 10-nm Tb₂₅Fe₇₅ nanoparticles for two scenarios: Tb atoms segregating to the surface (red dots) and to the center of a nanoparticle (green dots). σ is a width of concentration distribution defined as a Gaussian function.

- [2] M. Krupiński *et al.*, Phys. Rev. Mat., 5 (2021) 024405
- [3] R. F. L. Evans et al., J. Phys. Cond. Matt., 26:10 (2014) 103202

^[1] S. Mangin *et al.*, Nat. Mater., 13 (2014) 286

Contributed talk, Thu./19:30

Controlling the photoactivity of nanopatterned titanium oxide^{opane}

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Titanium oxide is a wide-bandgap semiconductor with high electron mobility, which makes it an excellent material for solar cells and photocatalytic reactions. The overall efficiency is a key parameter in this type of application, and one of the most effective ways of its increase is to maximize the working surface area of the active material, which can be done by nanopatterning. One of the most effective, scalable, and straightforward methods to synthesize nanopatterned titanium oxide is an electrochemical oxidation process called anodization. However, the order of the nanostructures obtained by this method is limited by the grain boundaries, which in turn affects the total surface area of the active material. To overcome this drawback, we used a combination of nanosphere lithography and anodization. The proposed approach allowed to obtain of TiO₂ nanotubes with long-range hexagonal ordering at large areas, as shown in Fig. 1.



Figure 1: The top view (left) and side view (right) show the surface morphology of anodized titanium oxide pre-patterned by nanosphere lithography.

The photoactivity of the TiO_2 nanotubes was studied by fluorescence spectroscopy in the UV-Vis range as a function of the patterning period and annealing temperature. The crystal structure of the nanotubes was characterized by X-Ray diffraction and Raman spectroscopy and compared to the material obtained by classical anodization. The fluorescence spectroscopy measurements revealed that the parameters of the patterning process have a strong influence on the photooxidation effect. These results indicate that the combination of pre-patterning and anodization provides an excellent tool for controlling their photoactivity.

Magnetic properties of copper-iron based composite particles kopane synthesized by laser melting in liquid

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Copper (Cu) is a well-known metal with highly useful physical and chemical properties, such as catalytic activity, high electrical and thermal conductivity or high corrosion resistance. Combining these features with magnetic properties of iron (Fe) into a composite promises multifunctionality desired for many applications. In our work, Cu (or CuO) and Fe₃O₄ colloid solutions were irradiated in various organic solvents by Nd:YAG laser with 2nd harmonic with various laser fluences and irradiation times. During laser melting in liquid process we can synthesize particles with different sizes, compositions or e.g. structures, even if we use the same starting compounds. This is possible due to a change in process parameters such as laser fluence, irradiation time, molar ratio of components or others, which strongly influences the final result. Differences in structure or chemical composition causes changes in properties, such as magnetic properties, which are the main topic of this work. Fig. 1b shows examples of magnetic hysteresis loops measured for different kinds of obtained particles. We can see that the presented hysteresis loops are different in parameters such as the coercive field, saturation magnetization or the shift of the hysteresis loop caused by the exchange bias effect, which in some cases can be strong and do not occur in other particles. This work gives us a method for obtaining complex particles, whose size, composition and magnetic properties can be controlled by the conditions of laser irradiation.



Figure 1: a) SEM image of one kind of obtained particles. b) Examples of magnetic hysteresis loops of obtained particles.

Acknowledgements: This work was supported by the Polish National Science Centre Program No. 2018/31/B/ST8/03043.

Contributed talk, Thu./20:00

Study of the structural, electronic, magnetic properties of MnCo₂Al Compound

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Structural, electronic, and magnetic properties of Co_2MnAl compound have been investigated using the first-principles calculations [1]. The electronic structures and magnetic properties of the Co_2MnAl compound with both Hg₂CuTi and Cu₂MnAl type structures are studied [2, 3].

It is found that the calculated lattice constants are in good agreement with the theoretical values. Using the general gradient approximation, we observe that the Cu₂MnAl-type structure is more stable than the Hg₂CuTi type. The Co₂MnAl compound were half-metallic ferromagnets in the Cu₂MnAl-type structure. The total magnetic moments of the Co₂MnAl compound in the Cu₂MnAl-type structure is 4 μ B. Furthermore, the origin for the appearance of the band gap in the Co₂MnAl compound was also discussed which shows them to be promising materials for possible spintronics applications.



Figure 1: Crystal cell of full Heusler structure.

- [1] W. Kohn *et al.*, Phys. Rev. A, 140 (1965) 1133
- [2] N. Xing et al., Comput. Mater. Sci., 45 (2009) 489
- [3] R. Mebsout et al., Int. J. Thermophys., 34 (2013) 507

SESSION VII: MULTIFUNCTIONAL MATERIALS

Chair: Wojciech Tabiś

8:30	Alessandro Surrente (Wrocław, Poland) Magnetically brightened dark excitons in two-dimensional metal	p. 46
9:00	Siham Benhabib (Paris, France) Photo-induced phenomena in quantum materials	p. 47
9:30	Naveen Kumar Chogondahalli Muniraju (Kraków, Poland) Incommensurate magnetic structure and multiple magnetic transi- tions in sawtooth lattice $BeCr_2O_4$	p. 48
9:45	Marian Cholewa (Rzeszów, Poland) Application of novel nanomaterials for development of radiation detectors	p. 49
10:00	Jaydeb Dey (Warszawa, Poland) Low-temperature spin arrangement in Mn ₂ GaC MAX phase film studied by Nuclear Magnetic Resonance	p. 50
10:15	Ana Marija Kožuljević (Zagreb, Croatia) Development of the novel positron emission tomography device based on single layer gamma-ray polarimeters	p. 51

Invaited talk, Fri./8:30

Magnetically brightened dark excitons in two-dimensional metal and halide perovskite nanoplatelets

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Perovskite nanoplatelets consist of Pb-halide-based octahedra planes, surrounded by large organic molecules. In this work, we determine quantitatively the splitting between optically dark and bright exciton states by performing magneto-optical spectroscopy in pulsed magnetic field up to 65 T of CsPbBr₃-based perovskites nanoplatelets with a number of lead-halide octahedra planes ranging from 2 to 4, schematically shown in Fig. 1a.



Figure 1: Top: schematic of crystal structure of lead-halide perovskite nanoplatelet. Bottom: spatial dependence of the band gap and the dielectric constant. b) Magneto-PL spectra of nanoplatelets. BX: bright exciton. DX: dark exciton. c) Measured bright-dark splitting as a function of nanoplatelet thickness. d) PL intensity ratio between dark and bright exciton states for the three nanoplatelet thicknesses investigated as a function of the applied magnetic field.

The brightening of the dark state induced in the Voigt configuration allows us to directly observe an enhancement of the PL signal related to optically dark species on the low-energy side of the spectrum, as we show in Fig. 1b. The measured dark-bright splitting is summarized in Fig. 1c. We also evaluate the ratio between the intensities of the magnetic field-brightened dark state and of the bright state. The experimental data can be fitted only by assuming a temperature of the excitons considerably larger than the lattice temperature, as shown in Fig. 1d. This suggests that at low temperatures the exciton population is not fully thermalized, which is indicative of the existence of a phonon bottleneck [1].

^[1] S. Wang et al., Nano Lett., 22 (2022) 7011-7019

Invaited talk, Fri./9:00

Photo-induced phenomena in quantum materials

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Quantum materials constitute a playground of interesting electronic and structural phases thanks to the various interplay between degrees of freedom. Controlling these phases in an out-of-equilibrium fashion leads to hidden phases that are unaccessible thermodynamically. Here I will discuss two examples of quantum materials, magnetite, and cuprates, which I investigated using two out-of-equilibrium techniques: ultrafast electron diffraction (UED) and time-resolved-Angle resolved Photoemission Spectroscopy (tr-ARPES). In this presentation, I will introduce ultrafast techniques and discuss the photoincluded effects in magnetite and cuprates. Magnetite undergoes an atypical metal-insulator transition in the neighborhood of 125 K known as Verwey Transition (VT). Here we use UED to trace the structural changes of magnetite across the VT under femtosecond pulsed light excitations. We used two excitations, 800 nm and 400 nm (1.6 and 3.09 eV, respectively). We distinguish two different time evolution of the strain depending on the excitation's energy. I will discuss the possible scenarios responsible for such differences in the ultrafast dynamic responses. The equilibrium tunning of doping, temperature, magnetic field, and pressure generates substantial changes in the electronic states of high $T_{\rm c}$ superconductors-cuprates. They undergo a gradual transition from Mott insulator to Fermi liquid with doping, crossing d-wave superconductivity, charge density wave, pseudogap, and strange metal phases. Usually, these changes are accompanied by an abrupt transformation in Fermi surface topology, the so-called Lifshitz transition. Two Lifshitz transitions have been demonstrated in cuprates, one on the underdoped side, corresponding to the Fermi surface reconstruction from hole arcs to electron pockets by the 2D charge density wave. The second is on the overdoped side, corresponding to the Fermi surface transformation from hole-like to electron-like crossing van Hove singularity. Light is demonstrated to be an efficient stimulus to control quantum matter's electronic and structural phases and induced hidden phases such as superconductivity, notably in cuprates. Here in this work, we address the effect of ultrashort pulses on the Fermi surface topology of high T_c superconductors cuprates $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212) by means time-resolved-Angle resolved Photoemission Spectroscopy (tr-ARPES) with a pump energy of 1.55 eV. For the first time, we demonstrate that high fluence pulses are significantly efficient in supplying the Fermi level with additional carriers through the photodoping process, driving non-adiabatically the Fermi surface from hole-like to electron-like. Surprisingly, we reveal that the induced Lifshitz transition is involved within a timescale of microseconds which is indicative of a long metastable state which can be probed by equilibrium techniques

Contributed talk, Fri./9:30

Incommensurate magnetic structure and multiple magnetic Zakopane transitions in sawtooth lattice $BeCr_2O_4$

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Single-phase multiferroics attract fundamental and technological interest because they combine switchable electric and magnetic polarization, and consequently, they offer the potential to cross-couple and positively impact the field of spintronics. $BeCr_2O_4$ belonging to the Pbnm space group with a sawtooth lattice is one of the earliest reported multiferroic compounds. In this work [1], we revisit this mostly unexplored material with a focus on multiple magnetic transitions at low temperatures. In this compound Cr (III) occupies the octahedral 4a site and Be (II) occupies the tetrahedral 4c site. This adopts a close packing structure with a 90° and 138° Cr–O–Cr bonds allowing for interesting magnetic superexchange interactions. In the present work, $BeCr_2O_4$ has been prepared using the solid-state reaction method and verified the phase purity and crystal structure using laboratory and synchrotron X-ray diffraction. The title compound displays three magnetic phase transitions at low temperatures at $T_{\rm N1} \approx 7.5$ K, at $T_{\rm N2} \approx 25$ K, and $T_{\rm N3} \approx 26$ K-revealed through magnetic susceptibility, specific heat, and neutron diffraction in this work. These magnetic phase transitions are found to be influenced by externally applied magnetic fields. Isothermal magnetization curves at low temperatures below the magnetic transitions indicate the antiferromagnetic nature with two spin-flop-like transitions occurring at $H_{c1} \approx 29$ kOe and $H_{c2} \approx 47$ kOe resulting in a complex field-temperature phase diagram. From neutron diffraction measurements we determined cycloidal spin structure in the temperature range $T_{\rm N3,N2} < T < T_{\rm N1}$, usually associated with electric polarization, thereby proposing the scenario of magnetism-driven ferroelectricity in $BeCr_2O_4$.

[1] H. C. Mandujano, Phys. Rev. B, 7 (2023) 024422

Contributed talk, Fri./9:45

Application of novel nanomaterials for development of radiation^{one} detectors

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A new class of nanomaterials has been investigated by the Author with collaboration with several groups for the SEE (secondary electron emission) properties and as candidate for highly efficient radiation detectors. The SEE yield of heterostructures of ZnO nanoneedles coaxially coated with AlN or GaN has been studied for the first time using electron, ion, and X-ray beams. The SEE yield of the heterostructures is enhanced significantly by the intrinsic nanostructure of the ZnO nanoneedle templates as compared to the AlN and GaN thin films on Si substrates. These findings open up a way to develop new universal highly efficient radiation detectors based on the SEE principle by incorporating these one-dimensional (1D) nanostructures as a material of choice. A similar idea was previously developed for carbon foils, boron-doped diamond and is now proposed for nanomaterials. Series of experiments have been performed with different radiation including electrons, ions and X-rays to better understand processes governing the SEE in 1D nanostructured materials. So far two international patents have been awarded for these works. Recently intensive works have been performed in collaboration with GSI in Darmstadt, Germany on 1D nanomaterials as possible candidates for radiation detectors for FAIR project.

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- [1] P. Boutachkov et al., Sci. Rep., 11 (2021) 737
- [2] M. Cholewa et al., Sci. Rep., 11 (2021) 10517
- [3] M. Cholewa et al., Phys. Status Solidi B, (2022) 2100445

J. Dey

Low-temperature spin arrangement in Mn₂GaC MAX phase film^{ane} studied by Nuclear Magnetic Resonance

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Mn₂GaC belongs to the family of $M_{n+1}AX_n$ (MAX) phase materials, grown as nanolaminated hetero-epitaxial thin films. This structure consists of Mn-C-Mn stacks interleaved with Ga-layers. The theoretical studies on Mn₂GaC indicated the presence of competing ferromagnetic (FM) and antiferromagnetic (AFM) interactions resulting at low temperatures in a complex magnetic structure, still calling for elucidation in view of the contradictory data reported in literature. To this end we performed the NMR study at 4.2 K on a 100 nm film of Mn₂GaC(0001)/MgO(111), applying the in-plane external magnetic field in the range from 0 to 6 T. The zero-field ^{69,71}Ga NMR experiments indicated the presence of non-collinear magnetic structure, which was further investigated by the in-field ⁵⁵Mn experiments. Such comprehensive approach allowed to conclude a helical spin structure with spins lying in hexagonal base plane, as shown in the Figure 1.



Figure 1: a) phase diagram of the identified magnetic structures as a function of exchange interactions between nearest (J_1) and next nearest Mn neighbors (J_2) ; b) schematic representation of the proposed helical magnetic structure at 4.2 K.

The helical period of this structure, extending along the *c*-axis, is incommensurate with the crystal lattice period. At higher values of B_{ext} , the moments lying in hexagonal base plane gradually align themselves towards B_{ext} , resulting in a gradual increase of the net magnetization, but a continuous distribution of orientations is still observed in the NMR experiment.

Acknowledgements: This work was supported by the National Science Center, Poland (grant number UMO-2019/35/B/ST3/03676).

Contributed talk, Fri./10:15

Development of the novel positron emission tomography device based on single layer gamma-ray polarimeters

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Positron emission tomography (PET) is a widely used imaging technique that exploits characteristics of positron annihilation. In this process, two gamma photons are emitted back-to-back with 511 keV energy and orthogonal polarizations. Present-day PET devices exploit the first two properties, but the measurement of the correlation in the polarizations is yet to be implemented and evaluated. Simulation studies have shown that the polarization measurements could improve the signal-to-noise ratio by suppressing the random background since it lacks correlations in polarization [1]. To test this, the concept of single-laver gamma polarimeters has been developed and examined [2]. The modules encompass scintillator matrices read out by silicon photomultipliers. We have studied and demonstrated that the modules can reconstruct the Compton scattering of the gamma ray even though they detect both the recoil electron and the scattered gamma in only one layer. It has also been demonstrated that correlations of the annihilation quanta can be deduced, and we have extensively studied both in-silico and in the laboratory the optimal detector configuration for achieving the highest polarimetric sensitivity [3]. To implement the polarization measurement in PET, we mounted four detector modules on the annular construction, which enables rotation around the annihilation source (Fig. 1 - left). Each detector module consists of four 8×8 crystal (GAGG:Ce and/or LYSO:Ce) matrices with either 2.2 mm or 3.2 mm pitch, which make 16 trans-axial rings with a total of 1024 pixels. We will report on the studies of the device's performance, focusing on the polarimetric measurements (Fig. 1 – right) both in laboratory tests and investigations with clinically relevant sources.



Figure 1: (left) PET device with the capability of measuring polarization correlations of an annihilation gamma photons. (right) Observed azimuthal difference distributions for GAGG:Ce modules mounted on the PET demonstrator device for $72^{\circ} < \theta_{1,2} < 90^{\circ}$.

- [1] A. McNamara et al., Phys. Med. Biol., 59 (2014) 7587
- [2] M. Makek et al., Nucl. Instrum. Methods Phys. Res. A, 958 (2020) 162835
- [3] S. Parashari et al., Nucl. Instrum. Methods Phys. Res. A, 1040 (2022) 167186

SESSION VIII: EXTREME LIGHT INFRASTRUCTURE AND MAGNETIC NANOMATERIALS

Chair: Henryk Fiedorowicz

11:00	Peter Dombi (Szeged, Hungary) Ultrasensitive optical probing of plasmonic hot electrons	p. 53
11:30	Gabriele Maria Grittani (Dolní Břežany, Czech Republic) Laser Plasma Electron Acceleration	p. 54
11:50	Eva Klimešová (Dolní Břežany, Czech Republic) Atomic, molecular and optical sciences at ELI Beamlines	p. 55
12:15	Jakub Jurczyk (Zaragoza, Spain) 3D nanolithography methods for novel spintronic devices	p. 56
12:45	Marcin Perzanowski (Kraków, Poland) Magnetization reversal process in exchange-biased thin films on anodized titanium oxide	p. 57
13:00	Arkadiusz Zarzycki (Kraków, Poland) Tunable Magnetic Schottky junction based on metallic oxide het- erostructure	p. 58

Zakopane

Invaited talk, Fri./11:00

Ultrasensitive optical probing of plasmonic hot electrons

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Non-thermal and thermal carrier populations in plasmonic systems raised significant interest in contemporary fundamental and applied physics. Although the theoretical description predicts not only the energies but also the location of the generated carriers, the experimental justification of these theories is still lacking.

Therefore, we demonstrated experimentally that upon the optical excitation of surface plasmon polaritons (SPPs), a non-thermal electron population appears in the topmost 4-6 nm domain of the plasmonic film directly coupled to the local fields [1]. The applied all-optical method is based on spectroscopic ellipsometric determination of the dielectric function, allowing us to obtain in-depth information on SPP-induced changes of electron occupancies (Fig. 1). The ultrahigh sensitivity of our method allows us to capture the signatures of changes induced by electron-electron scattering processes with ultrafast decay times. The experiments shed light on the build-up of plasmonic hot electron population in nanoscale media and establish the fundaments of future time-resolved experiments at ELI.



Figure 1: Setup for plasmonic hot electron probing with spectroscopic ellipsometry. These measurements are capable of accessing the dielectric function of the investigated system, the changes of which are in close correlation with the electron distribution function. (a) Retrieved and simulated differences between the dielectric function of the non-thermalized top layer (NT) and the thermalized part (T) of the gold film and (b) the corresponding electron occupancies for cw excitation.

Acknowledgements: We acknowledge the H2020 project "PetaCOM" and KKP137373 for support.

[1] J. Budai et al., Nat. Commun., 13 (2022) 6695

Zakopane

Contributed talk, Fri./11:30

Laser Plasma Electron Acceleration

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Electron accelerators are a cornerstone technology of modern society. They are used in their variations daily as strategic tools at the disposal of the healthcare system for medical imaging and cancer treatment. For example, medical linear accelerators already use electron beams up to 20 MeV for cancer radiotherapy. Radio-frequency acceleration is the backbone of the technology driving these machines and it is nowadays, after its first demonstration in 1928, generally acknowledged as an extremely reliable technology. Radio-frequency acceleration technology has nevertheless a fundamental limitation in their maximum achievable accelerating gradient to 100 MV/m that puts a constraint in terms of the size and, as a consequence, the cost. This inhibits the realization of compact accelerators as a source for free electron lasers, Thomson scattering x-ray sources, and high energy electron accelerators for radiotherapy. As of today, the only proven technology with the potential to overcome these limitations laser-plasma acceleration [1], which can withstand accelerating gradients exceeding 100 MV/mm. Its potential has in recent years motivated an extensive effort by numerous groups worldwide, leading to remarkable achievements, ranging from the demonstration of the first GeV laser-driven electron beams, to the acceleration of multi-GeV electrons via plasma guiding as well as to the demonstration of free electron lasing [2]. The desire to translate these exceptional results into working machines resulted in the demonstration of stable electron beam operation over more than 24 hours and the acceleration of quasimonoenergetic (QME) electron beams at 1 kHz repetition rate [3]. The experimental results and capabilities at ELI-Beamlines on laser plasma electron acceleration will be presented.



Figure 1: ALFA User Laser Plasma Electron Accelerator at ELI-Beamlines

- [1] E.Esarey et al., Rev. Mod. Phys., 81 (2009) 1229
- [2] W. Wang *et al.*, Nature, 595 (2021) 516
- [3] C. M. Lazzarini *et al.*, arXiv:2302.11415 (2023)

Contributed talk, Fri./11:50

Atomic, molecular and optical sciences at ELI Beamlines Zakopane

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ELI Beamlines facility is an international research center, operated within the Extreme Light Infrastructure ERIC, which offers femtosecond sources of photons and accelerated particles for user experiments. The MAC end-station at ELI Beamlines is a Multipurpose station for AMO (atomic, molecular and optical sciences) and CDI (coherent diffractive imaging) [1]. It is dedicated to investigations of ultrafast electron and ion dynamics in atoms, molecules and nanostructures employing synchronized XUV and NIR/Vis beams.

We review experimental capabilities, scientific opportunities and recent results at MAC. First, we present a detailed study of electron correlation dynamics in atomic krypton [2]. Employing a single high harmonic of the laser beam and synchronized NIR pulses with variable intensity we follow and control different electronic processes in the target.

We further move to the study of helium nanodroplets, which are relevant to radiation physics and chemistry of soft matter. Here we present results from investigations of interatomic Coulombic decay in pure and doped helium nanodroplets and studies of collective phenomena excited by laser pulses [3]. Altogether, we confirm that the advanced photon beams together with low density samples and available spectroscopic techniques at MAC can be used for leading research in the field of atomic, molecular and optical sciences.

- [1] E. Klimešová et al., Eur. Phys. J. Spec. Top., 11 (2021) 4183-4194
- [2] A. H. Roos et al., New J. Phys., 25 (2023) 013038
- [3] L. Jurkovičová et al., https://arxiv.org/abs/2301.10508

Invaited talk, Fri./12:15

3D nanolithography methods for novel spintronic devices Zakopane

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Recent advances in the fields of three-dimensional nanomagnetism and spintronics demands for the development of the novel methods of manufacturing of nanostructures with geometries beyond standard planar configurations. This has led to the rapid development of 3D micro and nanolithography methods such as focused electron or ion beam induced deposition (FEBID) or two-photon lithography [1].

In this contribution, we will present current developments in 3D nanolithography and its applications to 3D nanomagnetism. Advantages and limitations of 3D nanoprinting, sometimes in combination with thin film deposition methods and post annealing processes, to fabricate complex-shape magnetic structures such as (amongst others) helices, nano-trees, ramps and knots will be discussed [1, 2]. 3D shape-induced magnetic effects, such as the creation of topological stray fields [2] and domain wall auto-motion [3] will be presented. Moreover, different methods for magnetic characterization of the aforementioned structures will be shown.



Figure 1: Futuristic vision of an Internet-of-Things chip integrating 3D magnetic nanostructures.

Acknowledgements: This work was supported by the European Community under the Horizon 2020 Program, Contract No. 101001290 (3DNANOMAG).

- [1] A. Fernández-Pachecoet al., Nat. Commun., 8 (2017) 15756
- [2] C. Donnelly et al., Nat. Nanotechnol., 17 (2022) 136-142
- [3] L. Skoric et al., ACS Nano, 16 (2022) 8860-8868

Contributed talk, Fri./12:45

Magnetization reversal process in exchange-biased thin films on anodized titanium oxide

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Nanostructured magnetic materials have gained great interest due to their possible technological application in electronic or spintronic devices. The key issues which decides on the potential utilization of a material is the magnetization reversal process revealed by that system. One of the approaches to study the switching is the angular dependence of coercivity where the Kondorsky and Stoner-Wohlfarth models are often used as references. However, in many experimental reports angular dependencies of coercivity do not follow either of these formulas. Therefore, the question how the magnetization reversal takes place and how it is reflected in coercivity measurements is still one of the unsettled issues in the research on magnetic materials.

Here, we present our studies on the magnetization reversal process in the CoO/[Co/Pd] thin films exhibiting the exchange bias effect. Materials displaying this effect are considered promising candidates for industrial application. The system was deposited on a flat substrate and on an array of anodized titanium oxide nanostructures. The reversal mechanism was studied using a series of hysteresis loops measured for different angles Θ between the external field direction and the normal to the surface of a system (see Figure 1), and by First Order Reversal Curve method. The flat system shows a crossover between the reversal mechanism driven by the domain wall motion and the rotation of the magnetization. A similar situation takes place for the pattern sample. A factor which differs our results from other research on the reversal mechanism in flat and patterned systems is the presence of the interface exchange interaction, responsible for the exchange bias effect.



Figure 1: a) Exemplary hysteresis loops measured for the flat and patterned CoO/[Co/Pd] systems for various angles Θ . b) dM/dH distributions calculated from the loops. c) Angular dependencies of the coercivity field H_c (left scale) and the bias field H_{ex} (right scale).

Contributed talk, Fri./13:00

Tunable Magnetic Schottky junction based on metallic oxide^{akopane} heterostructure

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Junctions based on metal oxides are driving increased interest due to their unique properties and ability to consolidate electrical and magnetic effects in one device. Here, we focus on the electrical, magnetic and magnetotransport properties of Ti/Ti-O/Fe magnetic Schottky junctions, studied in a temperature range of 5-300 K and magnetic field of \pm 50 kOe. To prepare the junction, Ti layer was deposited on Si/Au substrate followed by partial oxidation of titanium using anodization. Then, Fe was deposited (Figure 1a) and the junction was annealed at 750 K.

The heterostructure was found to be an in-plane ferromagnet with two magnetic phases: the iron and iron oxide formed at the Fe/Ti-O interface. The effect of interatomic diffusion and mixing at the interface was confirmed with XRD and XPS.

The current-voltage characteristics present strong non-linear and temperature-dependent behavior of the Schottky diode where both Ti/Ti-O and Fe/Ti-O interface form the Schottky barrier. The Ti/Ti-O barrier shows a change of conductivity type from ohmic to Schottky type at around 250 K, which strongly influences the conducting performance of the junction. The conductivity of Ti/Ti-O/Fe depends on the magnetic field, voltage magnitude and voltage bias, providing the ability to control its transport properties. In particular, the positive magnetoresistance shows responsivity to the electric voltage polarization and its magnitude, which allows for tuning the electric properties of the oxide heterostructures (see Figure 1b and 1c).

Acknowledgements: This work was partially supported by the Polish National Science Centre with a grant 2015/19/D/ST3/01843.



Figure 1: a) Ti/Ti-O/Fe junction, b) magnetoresistance dependence on voltage bias, and c) voltage magnitude.

SESSION IX: PHYSICS FOR MEDICINE AND BIOLOGY

Chair: Joanna Czapla-Masztafiak Katarzyna Majzner (Kraków, Poland) 14:15Spectrophenotyping of leukemia cells – From Raman imaging to p. 60 diagnosis Jagoda Orleańska (Kraków, Poland) 14:45Raman-based study on biochemical changes in single endothelial p. 61 cells caused by antiretroviral drugs Patrycja Dawiec (Kraków, Poland) 15:00Raman spectroscopy in the diagnosis, classification, and monitorp. 62 ing of leukemia cells Giacomo Ubaldi (Bologna, Italy) 15:15Nuclear fragmentation cross section measurements with the FOOT p. 63 experiment Taoufik Lamrani (Katowice, Poland) 15:30The atomic-scale structure of pharmaceuticals amorphized by vit- p. 64 rification, cryo-milling, and pressure-densification

Invaited talk, Fri./14:15

Spectrophenotyping of leukemia cells – From Raman imaging to ane diagnosis

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Leukemia is a blood cancer that occurs as a result of genetic abnormalities in progenitor cells that disrupt the processes of differentiation and proliferation [1]. Particular types of leukemia can be distinguished on cell origin and molecular aberrations present in the cancer genome. In addition, some of these specific gene lesions defining leukemic subtypes can serve as predictive factors important for earlier disease detection, more accurate risk stratification, and treatment [2].

Recently, Raman imaging has been proposed as a potential tool that supports traditional leukemia diagnostic tests [1]. Raman spectroscopy (RS) belongs to analytical methods that, in a label-free and non-destructive way, are able to determine chemical composition in the sample. Raman imaging, due to the possibility of simultaneous detection of all cellular components with their spatial distribution, ensures a high level of selectivity and resolution and allows tracking metabolic changes in a single living cell, which is hardly possible with other methods.

Because the genetic lesions occurring in blasts affect the metabolism of cells and thus their biochemical composition, Raman spectroscopy appears to be an ideal tool for studying not only leukemic cells but also for classifying them. The developed Raman-based approach can be successfully applied for effective and automatic distinction between lymphocytes [3], leukemic cells with different genetic alternations [1], as well as for studies on the chemoresistance focused on identification of the mechanism of cell-drug interactions.

Acknowledgements: The "Label-free and rapid optical imaging, detection and sorting of leukemia cells" project is carried out within the Team-Net programme of the Foundation for Polish Science co-financed by the EU. Adrianna Wislocka-Orlowska is also acknowledged for her support in the measurements.

- [1] P. Leszczenko et al., Cancers, 13:21 (2021) 1-21
- [2] A. Pastorczak et al., Cancers, 13:7(2021) 1-25
- [3] A. Borek-Dorosz et al., J. Adv. Res., (2022)

Contributed talk, Fri./14:45

Raman-based study on biochemical changes in single endothelial cells caused by antiretroviral drugs

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Efavirenz (EFV) and etravirine (ETV) are highly active antiretroviral drugs used in HIV therapy. EFV and ETV are non-nucleoside reverse transcriptase inhibitors (NNRTI) that have a long plasma half-life and can be a source of drug-induced endothelial dysfunction, which in turn can lead to longterm increases in cardiovascular risk [1]. The steady-state high plasma concentration of EFV and ETV [2] has direct impacts on endothelial cells, which for<u>m the innermost part of blood vessels</u>. EFV was found to generate oxidative stress in endothelial cell lines [3] and has been associated with endothelial and cardiovascular dysfunction.

In this study, we present results from Raman-based studies on drug-induced changes caused by selected NNRTIs drugs on human aortic endothelial cells (HAECs). To follow in vitro biochemical changes caused by EFV and ETV, a confocal Raman microscope was applied. HAECs were incubated with EFV and ETV in a concentration of 1, 10 and 50 μ M for 24 h. Fixed cells were next imaged using the Witec Alpha 300 system. The Raman results revealed changes in the lipid composition, DNA/RNA content, and mitochondrial activity in drug-treated cells. Furthermore, for 10 μ M ETV-treated cells, it was possible to follow drug uptake and its distribution within perinuclear area.

In summary, Raman imaging combined with chemometrics enables monitoring of drug-induced biochemical changes in highly active antiretroviral therapy. Obtained results revealed that studied NNRTIs agents impacts on biochemistry of endothelial cells and allowed to identify molecular changes observed at subcellular level.

Acknowledgements: This work has been funded by the "Excellence Initiative – Research University" programme at the Jagiellonian University and supported by National Centre of Science (UMO-2016/21/D/ST4/00870 to KM and UMO-2018/29/B/ST4/00335 to MB).

- [1] E. L. Streck et al., Neurochem. Res., 36 (2011) 962-966
- [2] S. Vrouenraets et al., Expert Opin Pharmacother., 8 (2007) 851-871
- [3] M. Weiß et al., Cardiovasc. Toxicol., 161 (2016) 90-99

2023

Contributed talk, Fri./15:00

Raman spectroscopy in the diagnosis, classification, and monitoring of leukemia cells

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Analysis and understanding of the biochemical profile of single leukemia cells and their biology is crucial for the diagnosis and medical monitoring of patients. The research focusses on the development of Raman-based method that allows the molecular characterisation and tracking of changes in single cancer cells not only their specific and label-free identification, but also for monitoring of the effectiveness of pharmacological treatment (Figure 1).



Figure 1: The idea of Raman-based leukemia diagnostic approach using Raman imaging.

Using confocal Raman microscopy, a single cell chemical imaging was performed from tens of cells originating from different in vitro leukemia models. Identification of molecular differences between the in vitro systems was obtained through supervised and unsupervised chemometric analyses. As a result of the studies, molecular differences between normal and cancer cells were found. As a major source of distinction, changes in the intensity of bands assigned to nucleic acids, proteins, hemoproteins, and lipids were found. This proof-of-concept study shows that Raman imaging can be considered as a valid approach for developing label-free, objective, and automatic methods for the molecular and morphological classification of leukemia cells from patients.

Acknowledgements: The "Label-free and rapid optical imaging, detection and sorting of leukemia cells" project is carried out within the Team-Net programme of the Foundation for Polish Science co-financed by the EU. POIR.04.04.00-00-16ED/18-00.

Contributed talk, Fri./15:15

Nuclear fragmentation cross section measurements with the **FOOT** experiment

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Hadrontherapy is a medical treatment based on the use of hadron beams (usually protons and carbon ions) to treat deep-seated tumors on patients. According to how hadrons interact with matter, the dose release is low and almost constant in the entrance channel and increases sharply near the end of the path, called Bragg peak [1]. It overlaps the tumor region, sparing healthy tissues before and after it.

However, nuclear interactions occur for a fraction of the incoming particles, generating nuclear fragments that change the dose profile, so their effects must be taken into account in order to improve the treatment planning system.

Nuclear fragmentation has to be inspected even in the context of space radioprotection. Long-term human missions outside the Earth's orbit are being planned in the next years, including the NASA travels to Mars. It is then fundamental to preserve the astronauts health and to prevent electronics damage from exposure to cosmic radiation [2] and, in this scenario, the design and optimization of the spacecraft shielding requires a detailed knowledge of fragmentation processes.

At present, there is a lack of experimental data about nuclear fragmentation for light fragments (Z < 10) in the energy range between 100 MeV/n and 800 MeV/n, typical energies used in hadrontherapy and relevant for space radioprotection. To fill this data gap, the FOOT (Fragmentation Of Target) experiment [3] has been conceived with the main aim of measuring differential nuclear cross sections of both target and projectile fragments with an uncertainty smaller than 5%.

The FOOT experimental setups and the analysis procedure for a cross section measurement are shown, focusing on a 400 MeV/u 16 O beam on Carbon target data acquired at GSI (Darmstadt, Germany) in 2021.

- [1] W. D. Newhauser et al., Phys. Med. Biol., 60 (2015) R155
- [2] M. Durante et al., Rev. Mod. Phys., 83 (2011) 1245
- [3] G. Battistoni, Front. Phys., 8 (2020)

Contributed talk, Fri./15:30

The atomic-scale structure of pharmaceuticals amorphized by kopane vitrification, cryo-milling, and pressure-densification

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Low aqueous solubility of crystalline active pharmaceutical ingredients (APIs) is a critical challenge for drug development. Among the available approaches to improve the dissolution behavior of poorly water-soluble drugs, the amorphization process is an effective method for achieving better drug dissolution compared to their crystalline counterparts [1]. Various methods can be used to prepare noncrystalline forms of APIs, including quench cooling, spray drying, or mechanical treatment (milling, shearing, compression, etc.).

The atomic-scale structure of pharmaceuticals may differ when amorphized by the techniques mentioned above. It was demonstrated that the degree of intermolecular order could be tuned by proper thermodynamic conditions and mechanical stress when cryo-milled or pressurized [2, 3]. In this context, the results of structural characterization by the X-ray scattering technique and the pair distribution function will be presented in this contribution for selected pharmaceutical systems.



Figure 1: XRD patterns for cryomilled and vitrified itraconazole.

Acknowledgements: Authors acknowledge financial support by the National Science Centre (Poland), grant number: Opus 21 No. 2021/41/B/NZ7/01654.

^[1] B. C. Hancock et al., Pharm. res., 17 (2000) 397-404

^[2] D. Heczko et al., J. Phys. Chem. B, 124:52 (2020) 11949-11961

^[3] M. Rams-Baron et al., App. Phys. Lett., 111:12 (2017) 121902

SESSION X: MOLECULAR MAGNETISM

Chair: Beata Nowicka

16:15	Mark Meisel (Florida, USA) Materials in Metastable Forms – molecules to metals	p. 66
16:45	Dawid Pinkowicz (Kraków, Poland) Bringing molecular photomagnets to light – photochemical approach to molecular photomagnets	p. 67
17:15	Aleksandra Pacanowska (Kraków, Poland) Introduction of spin crossover compounds into electrospun fibres	p. 68
17:30	Pavlo Baloh (Košice, Slovakia) Experimental study of magnetic properties of $Dy(PO_3)_3$ glass	p. 69
17:45	Dominik Czernia (Kraków, Poland) The unconventional methods of tailoring magnetic properties in molecular magnets: proton and plasma treatments	p. 70

Zakopane

Invaited talk, Fri./16:15

Materials in Metastable Forms – molecules to metals

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An intense effort is being made to synthesize materials whose properties may possess new characteristics that allow their behaviors to be tuned by external stimuli. Three different approaches will be discussed and common themes will be highlighted.

Work being performed with the STM/STS team at Šafárik University in Košice, where external fields up to few tesla may be applied on samples cooled to 5 K, with Fe(II) spin-crossover samples provided by the Shatruk Group at Florida State University, will be presented. The local Fe(II) environment is a crucial aspect of this work [1].

Results of a pure and compositionally tuned alloy, CrMnFeCoNi, whose equiatomic composition is referred to as Cantor alloy, will be described. Experimental and DFT results indicate the overall importance of the local microscopic volume, influenced by the compositional neighborhood, in governing the strength and interaction of a local magnetic spin [2].

The High $B \times T$ (magnetic field times temperature) Facility will be described as part of a project to demonstrate the scalability of inductive heating processing of alloys in high magnetic fields. The results of growing pure Co from a Co-S flux in fields up to 9 T will be discussed, since Co liquid was cooled to a solid in field while being in the ferromagnetic state [3].

Acknowledgements: This work was/is supported by the European Microkelvin Platform, for the work at UPJŠ in Košice, the NSF via DMR-1708410, DMR-1852138, DMR-1644779 and DMR-2128556 (MagLab), the State of Florida, and by DOE EERE AMO DE-EE000913.

- [1] M. Gakiya-Teruya et al., J. Am. Chem. Soc., 143 (2021) 14563
- [2] T. A. Elmslie et al., Phys. Rev. B, 106 (2022) 014418, and arXiv:2208.09537.
- [3] C. L. Benyacko et al., Bull. Am. Phys. Soc., March (2023) D46.4, https://meetings.aps.org/Meeting/ MAR23/Session/D46.4

INVAITED TALK, FRI./16:45

Bringing molecular photomagnets to light – photochemical approach to molecular photomagnets

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Molecular photomagnets [1] can be designed and prepared via a bottom-up modular approach using low-energy preparation methods developed by coordination, organometallic or supramolecular chemistry, and crystal engineering with the support from physical and computational sciences. They belong to the class of molecule-based materials that become paramagnetic, ferromagnetic or simply change their magnetic properties upon illumination [2] – a feature hardly accessible in conventional solids – metal alloys or oxides.

Currently known photomagnetic compounds are merely laboratory curiosities due to the low operation temperatures below the boiling point of nitrogen in most cases [3]. Hence, the major goal of this field of research is the discovery of new strategies for room temperature (RT) photomagnets that would show light-induced ON/OFF ferromagnetic switching under normal conditions.



Figure 1: The concept of a molecular photomagnet – the paramagnetic state transforms into the magnetically ordered state upon illumination.

Acknowledgements: The project LUX-INVENTA has received funding from the European Research Council (ERC) under the European Union's Horizon Europe research and innovation program (grant agreement no. 101045004)

- C. Mathoniére *et al.*, Molecular Photomagnets. In Molecular Magnetic Materials (2017) (eds B. Sieklucka and D. Pinkowicz)
- [2] X. Qi et al., Angew. Chem. Int. Ed., 59 (2021) 3117
- [3] M. Magott et al., J. Am. Chem. Soc., 140 (2018) 15876

Contributed talk, Wed./10:15

Introduction of spin crossover compounds into electrospun fibresane

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In the field of multifunctional coordination frameworks, there has been much interest in developing processable materials of different shapes and sizes. The bistability and responsiveness to external perturbations offered by those molecule-based compounds make them promising candidates for the development of molecular switches and sensors. In response, different approaches have been undertaken to incorporate bistable molecular systems into flexible polymer matrices having in mind the need for future device integration.

In our research, we have focused on utilizing the electrospinning technique for the production of composite materials. As fillers two of the most popular spin crossover systems have been chosen – -iron(II)-triazole coordination complex obtained in the form of nanoparticles [1, 2] and 2D Hoffmann-type clathrate framework based on M(M = Pt, Ni) and Fe in the bulk form [3]. In fibre production, we have used polyvinylpyrrolidone (PVP) and poly(2-vinylpyridine – co–styrene) (P2VP-PS) into which we incorporated mentioned particles (Figure 1). With this approach, we were able to reproduce the switching abilities of both molecular systems in the obtained free-standing polymer composites.



Figure 1: Photograph, SEM image of electrospun fibres of P2VP-PS loaded with Pt-Fe Hoffmann-type clathrate. Right image: Comparison of magnetic susceptibility measurement of electrospun fibres to powder form.

Acknowledgements: This work was supported by the NCN within OPUS-22 Grant and by the NAWA agency under the STER and PROM Programs.

- [1] M. Gimenez-Marques et al., J. Mater. Chem. C, 3 (2015) 7946
- [2] R. Torres-Cavanillas et al., Dalton Trans., 48 (2019) 15465
- [3] V. Niel et al., Inorg. Chem., 40 (2001) 3838

Contributed talk, Fri./17:30

Experimental study of magnetic properties of $Dy(PO_3)_3$ glass kopane

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The studies of properties of magnetic ion-doped materials are mainly focused on the periodic and symmetrical crystal structures. The influence of the crystal field (CEF) which surrounds the magnetic ion in such case is uniform. Our study is focused on the amorphous phosphate glass doped with a Dy^{3+} ion which is conformed into a random network consisting of chains of PO₄ tetrahedra of various lengths to generate different CEF sets with a random distribution of energy levels.

The specific heat measurements of $Dy(PO_3)_3$ were performed in the range of 0.4-300 K in the magnetic fields up to 9 T. The low-temperature specific heat of disordered materials is characterized by a broad maximum commonly accepted as Boson peak (BP). The magnetic contribution dominates at the lowest temperatures, which overlaps the BP. Therefore, the specific heat of equivalent non-magnetic glass $Y(PO_3)_3$ was also measured at the same temperature range, revealing the BP at 12 K.

The magnetic susceptibility was measured from 1.8 K up to room temperature. An effective moment of 10.65 μ B was estimated, close to the theoretical prediction for Dy³⁺. Magnetization curves were measured in magnetic fields up to 5 T with temperatures ranging from 2 to 50 K.

X-band electron-paramagnetic resonance was measured from 0 to 1 T, revealing an additional absorption maximum at 100 mT. The maximum has the largest intensity at the same temperatures as the BP position in specific heat, implying a possible correlation.

Acknowledgements: This work was supported by the Slovak Research and Development Agency Project [grant numbers APVV-18-0197, APVV-SK-BY-RD-19-0008] and Scientific Grant Agency of the Ministry of Education, Science, Research and Sport of the Slovak Republic and the Slovak Academy of Sciences project VEGA 1/0132/22.

Invaited talk, Fri./17:45

The unconventional methods of tailoring magnetic properties in pane molecular magnets: proton and plasma treatments

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Consistent synthesis of new molecular compounds from building blocks is certainly one of the most prominent approaches to obtaining perspective materials. Moreover, the properties of molecular magnets are often sensitive to external stimuli such as temperature, pressure, light irradiation, or sorption of guest molecules which are well documented in the literature. Although not popular for magnetic materials, ion or plasma irradiation offer an alternative way to tailor the desired properties of the samples. In our work, we studied the effects of 1.9 MeV proton and plasma irradiation on the 2D coordination polymer based on nickel sulfate and a 1,3-phenylenediamine ligand (1), and three-dimensional cyanidebridged Nb(IV) and Mn(II) network (2), respectively. The samples of (1) and (2) after proton/plasma modification have been examined for structural and magnetic properties changes. For (1), the results show a possibility of tailoring magnetic hysteresis without changing Curie temperature. The general structure of (1) was preserved after proton irradiation, and only local changes were observed. For (2), a new phase with higher critical temperature appeared after plasma irradiation. During the presentation, I will show the challenges and difficulties related to such experiments and the possible advantages of using proton/plasma irradiation in molecular materials. Both methods offer unique ways of magnetic properties modification that may not be easily predicted, especially since they are not widely used in molecular magnetic materials.

Acknowledgements: This work was supported by the Polish Minister of Education and Science (grant No.: DI2017 006047).

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Poster No. 1

Contrast analysis of breast cancer in a mouse model using Zakopane non-targeted $NaDyF_4/NaGdF_4$ nanoparticles in MRI

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MRI provides the best soft tissue contrast when comparing with other diagnostic modalities. Relaxation times T_1 and T_2 of normal tissue and tumor create the contrast in MRI. Contrast agents shortening T_1 and T_2 relaxation times further improve detection of small pathologies such as early stages breast or brain cancers [1]. Furthermore, images can be post-processed to improve contrast. We studied changes in tumor contrast before and after non-targeted NaDyF₄/NaGdF₄ contrast injection. Then to further increase the contrast we applied an image subtraction.

We imaged a mouse with triple negative breast cancer (TNB) before and after an injection of a nontargeted NaDyF4/NaGdF4 nanoparticles (NP). We applied the IR RARE (T_1 -weighted), and MSME (T_2 -weighted) pulse sequences, using a 9.4 T MRI system. The results for the T_1 -w subtracted from the T_2 -w images showed that S_{tu} increased by 22%, the S_{ti} increased by 25% and C decreased 5%. We indicated that NaDyF₄/NaGdF₄ nanoparticles improved tumor contrast *in vivo* mouse imaging with TNB using T_1 -w MRI, and decreased contras in T_2 -w images. Further increase in contrast may be achieved by subtracting T_1 -w and T_2 -w images. We concluded that an image subtraction improved tumor contrast hence it may improve the accuracy of cancer detection.

Acknowledgements: This work was funded by the National Science Center, Poland. Grant number: OPUS 2018/31/B/ST5/03605.

[1] L. Smith et al., J. Nanomat., (2012) 1-7
Investigation of the optical and the electrical properties of $EuCd_2As_2$

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Magnetic topological materials, as a new category of topological materials, have attracted much recent attention. Recent work has shown that EuCd₂As₂ has a high density of magnetic moments, co-existing with a low concentration of itinerant carriers. Planes of Eu²⁺ atoms are separated by blocks of Cd₂As₂ which give rise to conduction and valence bands. Eu²⁺ atoms have large magnetic moments with J = 7/2, and they sit on the corners of a triangular lattice. The Fermi surface of EuCd₂As₂ appears to depend strongly on how the samples are grown [1, 2], with a delicate interplay of magnetism and the Fermi surface [2].

In the poster I will show optical measurements [3]. This will give an idea about the energy gap of EuCd2As2 and its band structure. Magnetization data using Squid will give information about the magnetic structure of this material. To address the Fermi surface and its shape we employ quantum oscillation in high magnetic field up 35 T.

- [1] J.-Z. Ma et al., Sci. Adv., 5 (2019) 4718
- [2] N. H. Jo et al., Nat. Comm., 12 (2021) 7169
- [3] D. Cottin *et al.*, "EuCd₂As₂: a magnetic semiconductor", arXiv:2301.08014 (2023)

Zakopane

Poster No. 3

Laboratory X-ray spectrometer at IFJ PAN

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Recent progress in development of laboratory X-ray sources, detectors and, most importantly, efficient X-ray optical systems made possible to implement X-ray techniques in laboratories and showed its potential wide application. A permanent laboratory-based setup offers the advantages of low costs and easy accessibility and, therefore, more flexibility in preparation and scheduling of the measurements.

Herein we present X-ray laboratory spectrometer setup for biological and chemical applications that was developed at the Institute of Nuclear Physics PAN in Krakow, Poland. X-ray laboratory spectrometer is characterized by unique combination of various X-ray techniques with biological and chemical laboratory on site that enables to design *in situ* and *in vitro* experiments performed on different material, including such complex systems as cells. <u>Offered X-ray techniques include X-ray</u> absorption and X-ray emission spectroscopy at high energy resolution employing wavelength-dispersive spectrometers. Available analysis enables studies of sample structure at atomic and molecular level. Thanks to the proposed technical developments, it is possible to do the measurements in the conditions mimicking physiological ones.

Examples of biological and chemical applications of the setup that include mostly studies of the electronic structure of metal complexes will be presented.

Acknowledgements: This work was partially supported by the National Science Centre (Poland) under Grant No. 2017/27/B/ST2/01890.

Zakopane

Poster No. 4

X-ray spectrum modification for multi-energy micro-CT

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Microscopic computed tomography (micro-CT) is one of the most common and versatile characterization tools in both life science research and industry, as it provides nondestructive, three-dimensional structural imaging of the sample with sub-micrometer resolution. However, one of the main drawbacks of micro-CT is a lack of contrast in imaging of low Z-number materials, which is especially critical for biological samples studies [1]. In recent years, multi-energy and spectral CT methodologies have emerged as potential candidates to address this challenge, but they usually require complex and high-cost modification of the imaging setup [2].

Herein, we demonstrate a novel approach to multi-energy micro-CT via modification of the X-ray beam spectral properties. Spectrum of the beam, generated by an X-ray tube, was altered by introducing various metal filters between the tube and a sample. In this way, multiple micro-CT datasets for the same sample were acquired with different incident X-ray beam properties. Next, a post-reconstruction data analysis algorithm was employed to enhance the contrast of the specific features of interest in the sample. The described multi-energy micro-CT technique is a straightforward and cost-effective approach to high contrast imaging of soft tissues, which is difficult to achieve in conventional micro-CT. In addition, it has a great potential to enable the quantitative analysis of constituents in the specimen, stained with common contrast agents or nanoprobes (e.g. gold nanoparticles).

Acknowledgements: We acknowledge National Science Centre, Poland (NCN) for support under grant no. $2020/37/{\rm B}/{\rm ST3}/00555$

- [1] E. Pauwels et al., J. Microsc., 250 (2013) 21-31
- [2] C. H. McCollough et al., Radiology, 276 (2015) 637-653

Switchable Molecular Materials Based on Coordination Clusters and

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Multifunctional molecular materials based on coordination scaffolds are in the spotlight of materials science in view of growing technological challenges dedicated to information storage, quantum computing and spintronics [1]. Invariably particular interest in research is focused on molecular materials combining several desirable physicochemical properties such as charge transfer, spin crossover or slow magnetic relaxations, to underly and shape switchable character controlled by external stimuli [2, 3].

Presentation will focus on results considering synthesis and physicochemical properties of bimetallic and trimetallic phases composed of variety clusters i.e., $\{M_x M'_{9-x} [W(CN)_8] (MeOH)_{24}\}$ (M, M' = Co,Fe, Mn, Ni; x = 0 - 9), $\{Fe_9[W(CN)_8]_x [Re(CN)_8]_{6-x} (MeOH)_{24}\}$ (x = 0 - 6), $\{Fe_9[W(CN)_8]_6 (L)_8\}$ $(L = Me_3 TACN)$. Synthesized materials represent different class of switchable magnetic properties: (i) slow magnetic relaxations and single molecule magnet behavior, (ii) spin crossover (iii) charge transfer.



Figure 1: Coordination skeleton of pentadecanuclear cluster $\{M_x M'_{9-x}[W(CN)_8](MeOH)_24\}$ (x = 0.9, M, M' = Fe, Ni, Co, Mn) with selected magnetic curves, which represent slow magnetic relaxations and spin transitions (CT / SCO).

- [1] J. Kobylarczyk et al., Coord. Chem. Rev., 19 (2020) 213394
- [2] J. Kobylarczyk et al., Dalton Trans., 49 (2020) 17321-17330
- [3] L. Shi et al., Cryst. Growth Des., 22 (2022) 3413-3420

POSTER NO. 6

Study on interaction and electronic structure of gold nanoparticles and hemin-based hybrid system using spectroscopic methods

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Effectiveness of current cancer diagnostics and therapy (theranostics) still need to be increased. Specialized nanosystems emerge as a novel tool in porphyrins delivery, which forms a theranostics path of cancer [1]. Plasmonic metallic particles and porphyrin can form a hybrid system to be the tool.

In this work, Au NPs and hemin, as a hybrid system elements, have been studied with ultraviolet visible (UV-VIS) and X-ray absorption spectroscopy (XAS) methods.

UV-VIS spectroscopy allowed defining Au NPs' and hemin's optical properties. AuNPs and hemin absorption shift registered by UV-VIS spectroscopy confirmed an interaction between them, however, is not sufficient proof for the hybrid system formation. XAS let us determine an electronic structure, chemical state, and density of states of hemin at different concentrations.

The determined Au NPs' and hemin's properties, structure, and registered interaction, form a solid background for further studies on porphyrins delivery nanosystems for cancer theranostics development.

Acknowledgements: This work was partially supported by the National Science Centre (Poland) under Grant No. 2020/37/B/ST3/00555.

[1] X. Xue et al., Bioconj. Chem., 30:6 (2019) 1585-1603

New 1,10-phenantroline- and imidazole-based dithienylethylene pane photoswitches – molecule profiling towards charge density studies

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One of main goals of chemistry and physics nowadays is to develop new materials that are able to respond rapidly and reliably to changes in local environment, and send out signals that let us know what is happening. It is crucial to be able to sensibly control the properties of such materials at the molecular level, so as to apply this knowledge to generate materials with particular properties across all the size scales from molecules to bulk materials, relevant for specific applications. Despite numerous efforts, this very challenging target remains far from being achieved.

In this context diarylethene (DAE) systems, especially the dithienylethene (DTE) derivatives (scheme below), appeared to be a very promising subject of investigations. The DTE fragment is capable of undergoing an intramolecular UV-light-induced pericyclic reaction. Furthermore, the reaction is most often fully reversible, when visible light is used. This makes such systems excellent molecular switches, which, in turn, can be utilized in molecular machines, as multi-state switches, or optical memory devices.

In this contribution we present new DTE-core-based molecules acting as photoswitches when irradiated with UV-Vis light. These can be readily traced with spectroscopic techniques both in solution and in the solid state. In addition, our initial attempts of in situ photocrystallography will be presented as well as material profiling studies allowing the experimental charge density investigations of newly-synthesized compounds.



Figure 1: Scheme of two-state dithienylethene (DTE) light-switchable system.

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X-ray photoelectron spectroscopy in analysis of Ti and Pd nanolayers

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X-ray photoelectron spectroscopy (XPS) is a surface analysis technique [1], in which a low energy X-ray beam is directed towards the studied sample, resulting in emission of electrons from the surface. Analysis of registered spectra of energy of the electrons gives information about such properties of surface as: qualitative and quantitative elemental composition, surface homogeneity and chemical environment of elements. The sensitivity of the XPS technique can be improved by applying the phenomenon of total reflection of X-ray radiation when the excitation beam is directed at the analyzed sample at an angle smaller than the critical angle. Such modified technique is known as the total reflection X-ray photoelectron spectroscopy (TRXPS) [2].

In presented study, XPS and TRXPS methods were applied in analysis of Ti (75 nm) and Pd (100 nm) nanolayers, deposited on Si substrate using physical vapor deposition (PVD) process. The measurements were carried out using XPS system (SPECS). In the TRXPS and XPS measurements both survey and detailed spectra (photoelectron peaks C 1s, N 1s, O 1s, Ti 2p, and Pd 3d) were investigated. Analysis of the TRXPS/XPS spectra concentrated on examination of the structure of the photoelectron peaks and, consequently, on determination of the binding energy of electrons, the intensity and FWHM of photoelectron peaks and the background level. It was shown, that the use of TRXPS geometry improves the detection limit of XPS technique.

Knowledge of the properties of Ti and Pd nanolayer surfaces will be applied in interpretation of the results of the studies carried out at the Institute of Physics of Jan Kochanowski University (JKU), related to the formation of nanostructures in the interaction of highly charged xenon ions with nanolayers [3].

- [2] A. Kubala-Kukuś et al., Spectrochim. Acta Part B, 145 (2018) 43-50
- [3] I. Stabrawa et al., Vacuum, 210 (2023) 111860

P. van der Heide, X-ray Photoelectron Spectroscopy: An Introduction to Principles and Practices, John Wiley & Sons, Inc., Hoboken, New Jersey, 2011

Sorption studies of electrospun composites

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Coordination systems showing responsiveness to various environmental stimuli and demonstrating measurable changes of their magnetic, electric or optical properties are perfect candidates for the construction of nanomaterials with potential application in electronic devices. $\{(NH_4)[Ni(cyclam)][Fe(CN)_6]$ $\cdot 5H_2O_n$ (NiFe) is a promising candidate because of its rare feature – multistability in room temperature. It undergoes metal to metal charge transfer accompanied by changes in structure, magnetic susceptibility and color in response to external parameters, such as temperature, humidity, pressure or light irradiation. As crystalline assemblies are brittle and susceptible to chemical corrosion in general, embedding them in organic polymers may help to prevent their degradation and improve their mechanical and surface properties. Selection of the suitable organic polymer as a base of the nanocomposite and optimalization of the preparation method have a key role in shaping the final properties of the resulting composite. We prepared electrospun composite mats based on poly(2-vinylpyridine) (P2VP) or poly(ϵ -caprolactone) (PCL) matrix with micro- and nanosized NiFe crystallites. Water sorption measurements show how different organic polymers can modulate water sorption properties of the nanocomposite.



Figure 1: SEM image of an electrospun composite mat and its water sorption isotherm in comparison to the isotherms of the components: P2VP and crystalline NiFe.

- $\left[1\right]$ M. Reczyński et~al., Angew. Chem. Int. Ed., 60 (2021) 2330
- [2] W. Sas et al., Magnetochemistry, 7 (2021) 61

Zakopane

Formation of calcium carbonate spherulites driven by coral Zakopane polyanionic protein

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Increased concerns about rising temperatures and ocean acidification are spurring scientists to investigate how it can affect the processes ensuring the survival of marine organisms. One of such vital processes is biomineralization, however, still little is known about the molecular mechanisms behind it.

Coral acid-rich proteins (CARPs) are postulated to be involved in the process of skeleton formation. So far, only four CARPs have been cloned and shown to induce the formation of aragonite crystals under conditions which do not allow for spontaneous precipitation [1].

Our goal is to elucidate what protein-mediated transient phases appear prior to the fully grown CaCO3 crystals, how are polyanionic proteins distributed within the crystals and what is their role in vitro in the formation of spherulitic structures of calcium carbonate, which were identified in the coral skeleton [2].

We cloned for the first time two novel CARPs from *Acropora millepora* [3] – secreted acidic protein 1A (SAP 1A) and aspartic and glutamic acid-rich protein (AGARP). By means of i.e. fluorescence correlation spectroscopy, confocal imaging and SEM we aim to decipher the early stages of the CARP-mediated nucleation pathway.

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- [1] T. Mass et al., Curr. Biol., 23 (2013) 1126-1131
- [2] C. Y. Sun *et al.*, ACS Nano, 11 (2017) 6612-6622
- [3] P. Ramos-Silva et al., Mol. Biol. Evol., 30 (2013) 2099-2112

Correlative Fluorescence and Soft X-ray Microscopy in the Waterne Window Region in an Integrated Lab-based Setup

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Multimodal imaging has emerged as an important tool for the life sciences, as a single method has proved insufficient for the holistic investigation of biological samples. Here we present a correlative soft X-ray (SXR) and fluorescence microscope that combines both methods in an integrated laboratory setup. This allows subsequent imaging without moving or altering the sample. Fluorescence microscopy provides functional contrast through labeling, but is not sufficient for comprehensive structural characterization of the sample. Correlation with SXR microscopy in the water window region (2.3 to 4.4 nm), which provides a high natural structural contrast in biological samples, is one way to fill this gap. This contrast is due to the strong absorption of carbon but relatively high transmission of water in this spectral region. Correlation of SXR and fluorescence microscopy has been realized at synchrotron radiation sources, but not in an integrated laboratory setup as presented here. We use a laser-generated plasma SXR source based on a double-stream gas puff target, which has been established for other X-ray and XUV imaging techniques. Using a Siemens star, we are able to demonstrate a resolution of 50 nm half pitch. For correlative imaging a wide field epifluorescence microscope including different filter sets has been integrated. The direct integration allows both modalities to be used sequentially without moving the sample. In addition, it is possible to quickly scan large areas of the sample with the fluorescence microscope to identify regions of interest for SXR microscopy. We demonstrate correlative imaging of fluorescent nanobeads, cyanobacteria, COS-7 cells and 3T3 cells.

Intrinsically disordered proteins involved in miRNA-mediated gene silencing – conformational dynamics, hydrodynamic properties and interactions

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Gene expression undergoes regulation at many levels. One of the regulation pathways takes place at the post-transcriptional level and involves microRNAs. These molecules are responsible for recognition and binding to an imperfectly complementary sequence at the 3' UTR of the targeted mRNA, which triggers a recruitment of a multiprotein machinery leading to the deadenylation and translation repression of the targeted mRNA. Elucidating the mechanism of the molecular interactions between these proteins has significant implications for our understanding of the miRNA-mediated gene silencing. The key biomolecule that is responsible for binding a CNOT1 subunit of the 3' CCR4-NOT deadenylase complex is the glycine and tryptophan rich protein of 182 kDa (GW182) [1]. The GW182-binding site of CNOT1 is yet to be identified. The C-terminal silencing domain (SD) of the GW182 protein is almost completely intrinsically disordered, except for the RNA Recognition Motif (RRM) [2]. GW182 SD is involved in molecular interactions with the subunits of the deadenylase CCR4-NOT complex. While the GW182 sequence motifs responsible for the interactions with the deadenylase complex have been characterized [3], a putative role of the RRM remains still elusive.

In this work, we present fluorescence correlation spectroscopy (FCS) studies of the hydrodynamic properties of a set of GW182 and CNOT1 protein variants. We estimate the binding affinity of various GW182 SD constructs. Our results unravel also how the presence of the RRM can influence the GW182 SD structural dynamics and thus could be involved in regulation of the GW182 SD interactions with CNOT1.

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- [1] J. Braun et al., Mol. Cell, 44 (2011) 120-133
- [2] M. K. Cieplak-Rotowska et al., J. Am. Soc. Mass Spec., 29 (2018) 158-173
- [3] M. R. Fabian et al., Nat. Struct. Mol. Biol., 18 (2011) 1211-1217

Crystal engineering of functional CN-bridged magnetic polymers characterized by elastic coordination networks

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Through the combination of appropriate building blocks, using the self-assembly method, it is possible to merge various physical properties in coordination systems, including sorption ability and magnetic order. The rational design and synthesis of structurally flexible molecular materials is often very challenging because of the need for precise control of the reaction conditions. Our research focus on the construction of coordination polymers by linking the cationic paramagnetic $[Ni(cyclam)]^{2+}$ complex with anionic octacyanidometallates(IV). It resulted, among others, in a series of porous 2D Ni-Nb honeycomb-like networks, which magnetic properties can be modulated by the type of guest s-block cations, as well as the amount of crystallisation water molecules present in the channels of the structure [1]. Furthermore, by reacting $[Ni(cyclam)]^{2+}$ with $[W(CN)_8]^{4-}$ under different conditions it was possible to obtain as many as six compounds of different dimensionality and topology (Figure 1) [2]. The factors determining the reaction pathway were temperature and addition of the lithium chloride electrolyte. These compounds constitute the largest family of CN-bridged networks obtained from the same pair of building blocks. For the 2D Ni^{II}-W^{IV} network of the honeycomb-like topology and its Ni^{II}-Mo^{IV} congener the photomagnetic effect was observed [3]. It was the first example of photo-magnetic switching of the $[M(CN)_8]$ ($M = W^{IV}$, Mo^{IV}) chromophores embedded into the Ni^{II}-based coordination polymers. Moreover, the photomagnetic response was found to be significantly stronger for the dehydrated phases of these compounds.



Figure 1: The scheme of reaction pathways between $[Ni(cyclam)]^{2+}$ and $[W(CN)_8]^{4-}$ building blocks leading to different topology CN-bridged networks.

- $\left[1\right]$ M. Heczko et~al., Dalton Trans., 50 (2021) 7537
- [2] M. Heczko et al., Inorg. Chem., 61 (2022) 13817
- [3] M. Heczko et al., Cryst. Eng. Comm., 21 (2019) 5067

The relaxation of the excited states of Cu⁺ complexes in their amorphous and crystalline phase environment

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Metalorganic copper complexes especially $[Cu(dmp)_2]^+$ (dmp = 2,9-dimethyl-1,10-phenanthroline) has been extensively studied as a model compound and possible building block for new photosensitizers. Recently $[Cu(dmp)_2]^+/[Cu(dmp)_2]^{2+}$ couple has also been successfully employed as a redox mediator in Dye Sensitized Solar Cells (DSSC) [1, 2]. Strikingly, solidified amorphous blends of multiple similar Cu^{+/2+} couples turned out to be excellent hole transporting materials [3] (HTM) reaching top efficiencies of solid state DSSC.

Interestingly, the HTM conductivity is severely limited by its crystallization. On one hand it was related to the restriction of structural flattering accompanying complex oxidation (Jahn-Teller distortion – JTD) but on the other hand, the limitation of JTD (by ligand modification in DSSCs comprising $[Cu(tmby)_2]^{+/2+}(tmby = 4,4',6,6'-tetramethyl-2,2'-bipyridine)$ was found to accelerate the kinetics of the electron transfer between the redox mediator and oxidized sensitizer [2]. The recalled apparently opposed interpretations could be justified by the existence of additional hindrance for structural changes in amorphous phase.

Assuming that the factors limiting complex's flattering are the same for JTD and pseudo-JTD (occurring after photoinduced metal to ligand charge transfer), we decided to study the dynamics of the excited electronic states of Cu^+ in crystalline Cu^+ and $Cu^{+/2+}$ as well as $Cu^{+/2+}$ in amorphous phase created in TiO₂ nanopores (analogically to DSSC). In our preliminary study on $[Cu(tmby)_2]$ we have found retardation of the sub-picosecond rise of 515 nm kinetics in amorphous phase (Fig.1) which could be related to pseudo-JTD. This interpretation needs further experimental evaluation, but supports our hypothesis. The study is ongoing.



Figure 1: Kinetics of transient absorption of $Cu(tmby)_2$ at 515 nm with the fitted time constants.

- [2] Y. Saygili et al., J. Am. Chem. Soc., 138 (2016) 15087-15096
- [3] M. Freitag et al., Energy Environ. Sci., 8 (2015) 2634-2637

^[1] M. Freitag et al., J. Phys. Chem. C, 120 (2016) 9595-9603

Magnon dispersion of CrI_3 under the influence of an external kopane magnetic field DMI orientation and temperature using atomistic spin dynamics

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As a prominent example of a two-dimensional (2D) van der Waals (vdW) magnet, CrI_3 has been studied intensively since its isolation in 2017. While there is a general consent that this 2D material is a non-Heisenberg compound holding different types of interactions (e.g., biquadratic exchange or Kitaev interactions), the exact nature of its magnetic character is still unclear. The opening of a band gap at the Dirac point on the magnon dispersion indicates topological features explained via a variety of models. Some groups contribute this topological gap to Kitaev interactions [1], while others assume Dzyaloshinskii–Moriya interactions (DMIs) are the main cause [2]. We simulate the magnon dispersion of CrI_3 via atomistic spin dynamics methods recently implemented in the Vampire code [3]. We consider a general spin Hamiltonian consisting of an isotropic Heisenberg exchange interaction, a DMI, a single ion magnetic anisotropy, and a biquadratic exchange. We study the system under different temperatures, magnetic fields, and sample orientations. We conclude that by changing the direction of the external magnetic field, we unveil the role of DMI interactions in the model.



Figure 1: Bands of the spin waves of CrI_3 monolayer at the temperature $T = 2/3 T_c$

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- [1] I. Lee et al., Phys. Rev. Lett., 124 (2020) 017201
- [2] A. Kartsev et al., npj Comp. Mat., 6 (2020) 150
- [3] R.F.L. Evans et al., J. Phys. Cond. Matt., 26:10 (2014) 103202

Improvement of prostate cancer contrast in MRI using complex pane nanoparticles

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Magnetic Resonance Imaging (MRI) has been used for early cancer detection and treatment monitoring due to its excellent soft tissue contrast [1, 2].

To further improve tumor contrast we have developed new core/shell NaDyF₄/NaGdF₄ nanoparticles changing both T_1 and T_2 relaxation times of surrounding water molecules. We also investigated toxicity, biodistribution and clearance of the new contrast agent. The relaxation times (T_1 and T_2) of the nanoparticles with various core/shell sizes and concentrations were measured at 9.4 T to find the optimum T_1/T_2 ratio for MRI. T_1 - and T_2 -weighted images using core/shell nanoparticles of the animal models of prostate cancer were collected and combined to provide enhanced contrast.

We imaged mice with prostate cancer before and after an injection of a non-targeted NaDyF₄/NaGdF₄ nanoparticle. We employed both an IR TrueFISP pulse sequence (T_1 -weighted images), and an MSME pulse sequence (T_2 -weighted images), using a 9.4 T MRI system.

Injection of non-targeted NaDyF₄/NaGdF₄ nanoparticle in a mouse with prostate cancer increases tumor contrast using IR TrueFISP (T_1 -weighted) pulse sequence comparing to no-contrast MRI.

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- [1] B. Blasiak et al., Mag. Res. Imag., 28 (2010) 784-9
- [2] B. Tomanek et al., Neuro-Oncology, 14:1 (2012) 53-63

Ab-initio study of chiral phonons

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Geometry of the compounds often allow the atoms to circulate around their equilibrium position in a circular or an elliptical trajectory. The phonons emerging from these kind of vibrations inherit the properties of its parent system and have a non zero value of angular momentum associated with them. We study the presence of chiral phonons in a system with orthorhombic symmetry (YalSi) [1], and also in systems with cubic Laves phases with chemical symbol ABi_2 (A = K, Rb, Cs). However, due to the presence of inversion symmetry, the total angular momentum is zero in all the mentioned system. We then artificially break the inversion symmetry by doping and propose and propose a new system with a non zero value of total Pseudo Angular Momentum (PAM) [2]. We study the dynamical stability of the final systems KRbBi₄, RbCsBi₄ and expect them to be used as platforms for studying phonon Hall effect.

- [1] S. Basak et al., Crystals, 12:3 (2022) 436
- [2] S. Basak et al., arXiv:2208.14041 (2022)

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