Book of abstracts

UWr-HZDR-CASUS

International Conference on Advanced Systems Research

CASUSCON

11-15 July 2022

Conference Venue

Wyndham Wrocław Old Town Hotel

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50-127 Wrocław, Poland

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Foreword

UWr- HZDR-CASUS International Conference on Advanced Systems Research

11-15 July 2022, Wrocław, Poland

The future belongs to those who believe in the beauty of their dreams.

Eleanor Roosevelt

It is our great pleasure to introduce to the readers the book of abstracts collected during UWr-CASUS-HZDR International Conference on Advanced Systems Research (CASUSCON). This publication contains nearly 50 presentations covering the whole variety of subjects wrapped by the conference widespread scope.

The aim of the conference is to provide a forum for discussion and bring together researchers in the field of broadly defined advanced systems. CASUSCON is an interdisciplinary event with main areas of interest including but not limited to the Matter, Energy, and Health and Life System Sciences. The event has drawn scientists from Poland and Germany, guests from the US, and the Czech Republic, as well as Max Born Symposium contributors.

The conference organizers acknowledge the valuable insights of all the experts who have contributed to the scientific content of the conference. We believe that the meeting will trigger effective scientific cooperation between the participants and their research groups from Wrocław scientific community, HZDR, and from the Czech Republic in the near future.

Eugeniusz Zych

Sebastian M. Schmidt

Conference Programme

UWr-HZDR-CASUS

International Conference on Advanced Systems Research

CASUSCON

11-15 July, 2022

Main building of the University of Wrocław (pl. Uniwersytecki 1)

Wyndham Wrocław Old Town Hotel, Św. Mikołaja 67 Street, 50-127 Wrocław

Monday, 11 July

Monday, 11 July	**Welcoming participants**	
	12:00-17:00	Registration at the hotel Wyndham Wrocław Old Town Hotel, Św. Mikołaja 67 Street
	18:00	Get together in the gardens of the General Consulate of Germany in Wrocław (Generalkonsulat Breslau), address: Podwale 76 Street

Tuesday, 12 July

Tuesday, 12 July	**Main building of the University of Wrocław, Aula Leopoldina, pl. Uniwersytecki 1**	
	Conference Opening	
	8:15	The conference reception is open
	8:45-9:00	**Robert Olkiewicz,** Rector of the University of Wrocław **Wojciech Murdzek,** Ministry of Education and Science **Cezary Przybylski,** Marshal of the Lower Silesian Voivodeship
	9:00-9:10	**Sebastian M. Schmidt**, Helmholtz – Zentrum Dresden – Rossendorf - An International Research Center in the Heart of Europe
	9:10-9:20	**Eugeniusz Zych**, We can do it. Together.
	9:20-10:40	**Session 1**
	9:20-9:40	Invited talk I-1 **Piotr Ponikowski**, *Title not provided*

	9:40-10:00	Invited talk I-2 **Anna Czyż**, New Era of Targeted Therapy in Hematooncology - the Role of Advanced Systems Research
	10:00-10:20	Invited talk I-3 **Tyll Krüger**, Households as Structural Risk Factors in Epidemic Dynamics
	10:20-10:40	Invited talk I-4 **Michael Bussmann**, CASUS - A German-Polish Institute for Data-Driven Systems Science
	Wyndham Wrocław Old Town Hotel	
	10:40-11:30	**COFFEE BREAK**
	11:30-13:10	**Session 2**
	11:30-11:50	Invited talk I-5 **Urlich Schramm**, Applications of Compact Laser Plasma Particle Accelerators in Health and Basic Research
	11:50-12:10	Invited talk I-6 **Mechtild Krause**, Biomarker for Treatment Stratification in Radiooncology
	12:10-12:30	Invited talk I-7 **Artur Yakimovich**, Machine Learning In Biomedical Images to Study Infection and Disease
	12:30-12:50	Invited talk I-8 **Aleksander Czogalla**, Complex Behavior of Signaling Lipids Within Membranes
	12:50-13:10	Invited talk I-9 **Karim Fahmy,** Membrane Protein Hydration is Linked to Membrane Lateral Pressure In Copper Transport
	13:10-14:30	**LUNCH BREAK (on your own)**
	14:30-16:10	**Session 3**
	14:30-14:50	Invited talk I-10 **Katrin Pollmann**, Biohydrometallurgical Concepts for Metal Recovery from Primary and Secondary Resources

Tuesday, 12 July	14:50-15:10	Invited talk I-11 **Cornelius Fischer**, Numerical and Analytical Concepts of Reactive Transport Towards Prediction of Contaminant Migration in the Subsurface
	15:10-15:30	Invited talk I-12 **Sascha Heitkam**, Optimizing the Froth Zone in Mineral Flotation and Adsorptive Bubble Separation
	15:30-15:50	Invited talk I-13 **Agnieszka Beata Kuc**, Simulation of Hydrogen Species Diffusion Between Layers of 2D Materials
	15:50-16:10	Invited talk I-14 **Joachim Wosnitza**, Materials Research at the Dresden High Magnetic Field Laboratory
	16:10-16:40	**COFFEE BREAK**
	16:40-18:20	**Session 4 – Max Born Symposium**
	16:40-17:00	Invited talk I-15 **Pasi Huovinen**, Centre for Simulations of Superdense Fluids
	17:00-17:20	Invited talk I-16 **Daniel Bemmerer**, Experimental Nuclear Astrophysics at Felsenkeller Underground Laboratory
	17:20-17:40	Invited talk I-17 **Tomasz Pawłowski,** Early Universe Evolution from Loop Quantum Cosmology
	17:40-18:00	Invited talk I-18 **Ralf Schützhold**, Theory of Non-Equilibrium Phenomena
	18:00-18:20	Invited talk I-19 **Jan T. Sobczyk**, Neutrino Physics and Monte Carlo Simulations
	19:00	Networking dinner in the Botanical Garden of the University of Wrocław (address: Sienkiewicza 23 Street)

Wednesday, 13 July

Wednesday, 13 July	Wyndham Wrocław Old Town Hotel	
	9:00-11:00	**Session 5**
	9:00-9:20	Invited talk I-20 **Sławomir Prucnal**, Modification of Optoelectronic Properties of TMDC Monolayers by Ion Implantation
	9:20-9:40	Invited talk I-21 **John Michael Klopf**, ELBE: An Accelerator Driven Radiation Source at its Best
	9:40-10:00	Invited talk I-22 **Shavkat Akhmadaliev**, Materials Science with Ion Beams at the HZDR's Ion Beam Center
	10:00-10:20	Invited talk I-23 **Martin Rudolph**, Improvements of the Fine Particle Separation by Means of Froth Flotation with a Special Focus on Local Polymetallic Resources
	10:20-10:40	Invited talk I-24 **Kerstin Eckert**, Bubbles, Surfactants, Particles: Fluid Dynamics Aspects of Resource Technologies
	10:40-11:00	Invited talk I-25 **Pavel Evtushenko**, DALI - HZDR Next-Generation IR-THz VUV Photon Source for Ultrafast Science
	11:00-12:00	**COFFEE BREAK and POSTER SESSION**
	12:00-13:40	**Session 6**
	12:00-12:20	Invited talk I-26 **Maksym Buryi**, Challenges in the Synthesis of Nanomaterials with the Required Properties
	12:20-12:40	Invited talk I-27 **Thomas Heine**, Digital Chemistry for the German Excellence Strategy: Dresden-Erlangen Center for Digital Chemistry (DEDICHEM)
	12:40-13:00	Invited talk I-51 **Rico Friedrich**, Data-driven design of two-dimensional non-van der Waals materials

Wednesday, 13 July	13:00-13:20	Invited talk I-28 **Michael Hecht**, Multivariate Interpolation in Non-Tensorial Nodes Lifts the Curse of Dimensionality for Trefethen Functions
	13:20-13:40	Invited talk I-29 **Zhandos Moldabekov**, Excitations of an Inhomogeneous Electronic System: From Ambient Conditions to Warm Dense Matter
	13:40-15:00	**LUNCH BREAK (on your own)**
	15:00-17:00	**Session 7**
	15:00-15:20	Invited talk I-31 **Christian Richter**, Proton Therapy: Today and in the Future
	15:20-15:40	Invited talk I-32 **Krzysztof Kałwak**, CAR-T Cells in Pediatric Patients with Leukemia and Solid Tumors. Current Status and Future Perspectives
	15:40-16:00	Invited talk I-33 **Bartosz Helfer**, Why Meta-Research is Important and Can We Make It More Efficient?
	16:00-16:20	Invited talk I-34 **Mariusz Ptak,** Numerical Models of the Human Brain
	16:20-16:40	Invited talk I-35 **Paweł Błażej**, Some Theoretical Aspects of Reprogramming the Standard Genetic Code
	16:40-17:00	Invited talk I-36 **Małgorzata Bogdan**, Regularization Techniques in the Analysis of Large Data Sets
	19:00	Conference dinner at Hotel Wyndham Wrocław Old Town

Thursday, 14 July

Thursday, 14 July	**Wyndham Wrocław Old Town Hotel**	
	9:00-11:40	**Session 8 - Max Born Symposium**
	9:00-9:20	Invited talk I-37 **Attila Cangi**, Data-Driven and Physics-Informed Modeling of Matter Under Extreme Conditions
	9:20-9:40	Invited talk I-38 **Gerd Röpke**, Correlations in Dense Matter
	9:40-10:00	Invited talk I-39 **Pok Man Lo**, Probing of the QCD Phase Boundary Within Heavy Ion Collisions
	10:00-10:20	Invited talk I-40 **David Blaschke**, Matter Under Extreme Conditions in Neutron Stars and Their Mergers
	10:20-10:40	Invited talk I-41 **Naser Ahmadiniaz**, Observability of Coulomb-Assisted Quantum Vacuum Birefringence
	10:40-11:00	Invited talk I-42 **Matthias Kaminski**, Quantum dynamics far from equilibrium
	11:00-11:20	Invited talk I-43 **Tobias Dornheim**, Frontiers of Computational Quantum Many-Body Theory
	11:20-11:40	Invited talk I-44 **Kay Potzger**, Tuning Magnetic Properties by Introducing Defects
	11:40-13:00	**LUNCH BREAK (on your own)**
	13:00-14:20	**Session 9**
	13:00-13:20	Invited talk I-45 **Krzysztof Sośnica**, Space and Satellite Research at UPWr
	13:20-13:40	Invited talk I-46 **Wojciech Bożejko**, Discrete Optimization in the Era of Quantum Computing - a Case Study

Thursday, 14 July	13:40-14:00	Invited talk I-47 **Witold Rohm**, Human and Animal Mobility - Integrated Science of Movement at UPWr SpaceOs
	14:00-14:20	Invited talk I-48 **Justin Calabrese**, Animal Movement Research as a Cross-Cutting Theme at CASUS
	14:20-15:00	**COFFEE BREAK**
	15:00-16:20	**Session 10**
	15:00-15:20	Invited talk I-49 **Małgorzata Werner**, Air pollution and allergenic pollen - integrated approach to modelling, measurements & health effects
	15:20-15:40	Invited talk I-50 **Martin Nikl**, *Title not provided*
	15:40-16:00	Invited talk I-30 **Marin Bukov**, Self-Correcting Quantum Many-Body Control Using Reinforcement Learning With Tensor Networks
	16:00-16:20	Invited talk I-52 **Przemysław Gagat,** Screening Proteomes for Prediction and Design of Antimicrobial Peptides with AmpGram
	16:20-16:35	**Closing remarks from organizers**

Friday, 15 July

Friday, 15 July	
	Departure

Abstracts

in the Programme order

I-1

TITLE NOT PROVIDED

P. Ponikowski*

Wroclaw Medical University, Wyb. Pasteura, 50-367 Wroclaw, Poland

* corresponding author: *piotr.ponikowski@umw.edu.pl*

Abstract not provided.

I-2

A NEW ERA OF TARGETED THERAPY IN HEMATOONCOLOGY - THE ROLE OF ADVANCED SYSTEMS RESEARCH

A. Czyz[1,*]

[1]*Department of Hematology and Bone Marrow Transplantation, Wroclaw Medical University, Wroclaw, 50-357, Poland*

* corresponding author: *a.czyz@ umw.edu.pl*

Keywords: molecular targeted therapy**,** targeted immunotherapy, CAR-T cells, hematological malignancies, acute leukemia, lymphoma, big data analysis, artificial intelligence, learning machines

Emerging high-throughput technologies, including next-generation sequencing (NGS) and microarrays, which enable the analysis of individual genomes, epigenomes, and transcriptomes have brought great advances in understanding biology and heterogeneity of hematological malignancies [1,2]. Nowadays, genomics has become an integral part of hematooncology providing diagnostic, prognostic, and therapeutic values in acute myeloid leukemia (AML), myelodysplastic syndromes, aggressive lymphomas or acute lymphoblastic leukemia (ALL) [1,2,3]. Widening knowledge on the biology of hematological malignancies resulted in the development of a broad spectrum of molecular targeted agents. In addition, growing understanding of the phenomenon of tumor escape from immune surveillance led to approval of immune check point inhibitors (CPIs) and further development of targeted immunotherapy, including bi-specific antibodies and chimeric antigen receptor (CAR) T cell therapy, initiating a new era of chemo-free therapy of hematological malignancies. Genetics already play a significant role in decisions related with hematopoietic stem cell transplantation (HSCT) [1], and increasingly influence the selection of targeted therapies [4,5]. High-throughput technologies and patient-generated health data provide the enormous amount of unprecedented complexity picture [2,3]. Clinicians are therefore faced with the challenge how to make the best use of the surfeit of biological data available to them to optimize the choice of these innovative therapies. Artificial intelligence (AI) may help to predict responses to targeted therapy using established biomarkers and may be used to search for new alternative biomarkers, including "omics" [3,4]. For example, in a registry study, Shouval et al. developed a model for prediction of 100-day mortality following allogeneic HSCT [3]. Then as well, AI could be used to build predictive/prognostic models for CPIs and CAR-T cell therapy, as shown in early studies in the field [4,5].

In summary, as high-throughput technologies such as NGS and sequencing whole genome, whole exome and whole transcriptome (WGS/WES/WTS) will be feasible for routine use in the next few years, AI-supported decision systems will therefore become a part of clinical practice in a new era of targeted therapies in hematological malignancies.

[1] L. Bullinger, *J. Clin. Oncol.* **35** (2017) 934.

[2] T. Haferlach, *British J. Hematol.* **188** (2020) 36.

[3] R. Shouval, *British J. Hematol.* **192** (2020) 239.

[4] F. Huemer, *Int. J. Mol. Sci.* **21** (2020) 2856.

[5] L. Vercellino, *Front Oncol.* (May 28 2021) doi: 10.3389/fonc.2021.664688

I-3

HOUSEHOLDS AS STRUCTURAL RISK FACTORS IN EPIDEMIC DYNAMICS

T. Krüger*

Wroclaw University of Science and Technology, Wyb. Wyspiańskiego 27, 50-370 Wroclaw, Poland

* corresponding author: *tyll.krueger@pwr.edu.pl*

Abstract not provided.

I-4

CASUS – A GERMAN-POLISH INSTITUTE FOR DATA-DRIVEN SYSTEMS SCIENCE

M. Bussmann*

Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

* corresponding author: *m.bussmann@hzdr.de*

Abstarct not provided.

I-5

APPLICATIONS OF COMPACT LASER PLASMA PARTICLE ACCELERATORS IN HEALTH AND BASIC RESEARCH

U. Schramm[1,2,*]

[1]*Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany*
[2]*Technische Universität Dresden, 01062 Dresden, Germany*

* corresponding author: *u.schramm@hzdr.de*

Keywords: laser plasma advanced accelerators

The application of laser plasma accelerated proton beams [1] in radiation therapy of cancer has been proposed and discussed almost since the first demonstration of plasma accelerators reaching 10s of MeV energies. It was initially motivated by accelerator compactness and consequently assumed cost efficiency, promising a wider spread of advanced therapy methods. Various and still ongoing in-vitro studies have been performed to investigate the radiobiology of these intense particle bunches, in particular with respect to the exploration of potential dose rate related effects. With the recently reported FLASH effect, a high dose rate effect observed to reduce radiation toxicity in normal tissue, the field has regained significant interest as provision of high single pulse dose rate is inherent to plasma accelerators. For the translation to in-vivo studies laser accelerated proton beams however not only lacked sufficient energy to penetrate the required volume but often stability and reprodicibility of beam parameters to ensure the provision of a homogeneous dose distribution in a prescribed way. This presentation focuses on the development at the Petawatt laser DRACO at Helmholtz-Center Dresden-Rosendorf and the related reference accelerators in use a spart oft the Dresden Platform that enabled the dose controlled systematic irradiation of tumors in mice [2] with laser accelerated protons. Details on acceleration mechanisms and strategies to increase stability and energy well beyond the 60 MeV range are discussed [3] as well as beam transport by means of a dedicated pulsed solenoid beamline to a secondary target together [4] with online metrology and dosimetry. Dose profiles reached for the first mouse irradiation campaign [2] are reported as well as future perspectives for FLASH related studies.

[1] F. Albert, et al., *New Journal of Physics* 23, 031101 (2021)
[2] F. Kroll, et al., *Nature Physics* 18, 316 (2022)
[3] T. Ziegler, et al., *Scientific Reports* 11, 7338 (2021)
[4] F. Brack, et al., *Scientific Reports* 10, 9118 (2020)

I-6

BIOMARKER FOR TREATMENT STRATIFICATION IN RADIOONCOLOGY

M. Krause*

Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

* corresponding author: *m.krause@hzdr.de*

Abstract not provided.

I-7

MACHINE LEARNING IN BIOMEDICAL IMAGES TO STUDY INFECTION AND DISEASE

A. Yakimovich[1,*]

[1]*CASUS - Center for Advanced Systems Understanding, Helmholtz-Zentrum Dresden-Rossendorf e.V. (HZDR), Untermarkt 20, 02826 Görlitz*

* corresponding author: *a.yakimovich@hzdr.de*

Recent advances in Machine Learning (ML) and Deep Learning (DL) are revolutionizing our abilities to analyze biomedical images and deepen our understanding of infection and disease. Among other host-pathogen interactions may be readily deciphered from microscopy data using convolutional neural networks (CNN). ML/DL algorithms may allow unambiguous scoring of virus-infected and uninfected cells in absence of specific labeling. Furthermore, accompanied by interpretability approaches, the ability of CNNs to learn representations, without explicit feature engineering, may allow uncovering yet unknown phenotypes in microscopy. One such example is our recent tandem segmentation-classification algorithm aimed to uncover morphological markers of *Caenorhabditis elegans* lifespan and motility.

I-8

COMPLEX BEHAVIOR OF SIGNALING LIPIDS WITHIN MEMBRANES

A. Czogalla[1,*], J. Żelasko[1], D. Drabik[1]

[1]Department of Cytobiochemistry, Faculty of Biotechnology, University of Wrocław, ul. F.Joliot-Curie 14a, Wrocław, 50-383, Poland

* corresponding author: *aleksander.czogalla@uwr.edu.pl*

Keywords: signaling lipids, model membrane systems, lipid-lipid and protein-lipid interactions

Lipids are fundamental structural components of biological membranes. In addition, they are essential for a wide range of cellular functions, such as signal transduction. Until recently, lipidprotein recognition was considered as ligand-receptor events, based largely on specific interactions of proteins with lipid head groups. Each of signaling lipids (e.g. phosphatidic acid, PA) may be involved in a broad array of cellular pathways, which suggests that their biological activity is precisely regulated. While the local action of numerous specific lipid-metabolizing enzymes control levels and turnover of signaling lipids, additional molecular mechanisms are necessary to fine-tune protein-lipid recognition [1]. Lipid composition, bilayer organization/topography and the presence of specific ions can lead to changes of lipid head group conformation, its exposition to the water-bilayer interface and/or domain formation. In a consequence, these and other factors stay behind lipid recognition by peripheral membrane
proteins – a concept known as lipid presentation [2].
In our study we employ a broad range of membrane model systems, including lipid monolayers and vesicles of different size to analyze how signaling lipids behave in bilayers of different composition and in variable conditions and how peripheral membrane proteins selectively recognize individual signaling lipid species. Using state-of-the-art biophysical approaches together with molecular dynamics simulations, we elucidated molecular mechanisms that modulate the behavior of signaling lipid and their recognition. This led us to discover that the structure of acyl chains strongly influences behavior of PA [3], which is reflected by altered recognition of the lipid by peripheral proteins [4]. Also, cholesterol appeared to be a potent modulator of lipid presentation in case of PA and other lipids (e.g. phosphatidylinositides), although the consequences to protein membrane recruitment and/or activation most probably strongly depend on structural features of membrane-binding domains. This suggests that within a cell several subspecies of a particular signaling lipid may play different roles.
Our results allow to decode the mechanisms, by which signaling lipids are selectively recognized by effector proteins. This is crucial to understand cellular signaling pathways and consider additional, so far poorly defined aspects of their regulation and mutual relationships.

[1] Zegarlińska J., Piaścik M., Sikorski A.F., Czogalla A. (2018). Phosphatidic acid - a simple phospholipid with multiple faces. *Acta Biochim Pol.*, 65,163-171; [2] Czogalla A., Grzybek M., Jones W., Coskun U. (2014). Validity and applicability of membrane model systems for studying interactions of peripheral membranę proteins with lipids. *Biochim Biophys Acta*, 1841, 1049-1059; [3] Drabik D., Czogalla A. (2021). Simple Does Not Mean Trivial: Behavior of Phosphatidic Acid in Lipid Mono- and Bilayers. *Int J Mol Sci*, 22, 11523; [4] Żelasko J., Czogalla A. (2022). Selectivity of mTOR-Phosphatidic Acid Interactions Is Driven by Acyl Chain Structure and Cholesterol. *Cells*, 11, 119

I-9

MEMBRANE PROTEIN HYDRATION IS LINKED TO MEMBRANE LATERAL PRESSURE IN COPPER TRANSPORT

L. Nucke[1], Y.H. Huang[1], A. Sayed[1], M. Hof[2], K. Fahmy[1,*]

[1]Helmholtz-Zentrum Dresden-Rossendorf, k.fahmy@hzdr.de, Bautzner Landstrasse 400, 01328 Dresden, Germany
[2] J. Heyrovsky Institute of Physical Chemistry, martin.hof@jh-inst.cas.cz, Dolejškova 2155, Libeň, 182 00 Praha 8, Czech Republic

* corresponding author: *k.fahmy@hzdr.de*

Keywords: ion transport, membrane protein, lipid protein interaction, protein hydration

We have used the copper-ATPase LpCopA from *Legionella pneumophila*[1]as a model system to study intra-membrane protein hydration. Time-resolved fluorescence spectroscopy of the dye BADAN linked to the conserved copper-binding transmembrane CPC motif revealed substantial mobility of internal water in detergent, whereas dipol mobility was restricted in lipid nanodiscs (NDs) with remarkably distinct responses of the two cysteines. Functionally required lipid protein interactions thus shape an intra-membrane protein gradient of water mobility in the ion transporter as opposed to the more hydrated but non-functional detergent-solubilized protein.[2] These dipolar relaxation studies of BADAN report water mobility only, whereas the amount of intra-membrane protein was determined by osmotic pressure-dependent static fluorescence of BADAN. We show that CopA undergoes large volume changes that correspond to a pressure-induced release of water molecules in the detergent-solubilized state. In NDs, membrane lateral pressure reduces the effect on further water release by osmotic pressure. The data demonstrate that transient hydration / dehydration events during catalytic activity will be opposed or supported by lateral pressure, respectively, rendering the elastic membrane properties a transient reservoir for free enthalpy in the catalytic cycle.

[1] P. Gourdon, P. et al. *Nature* **475** (2011) 59.
[2] E. Fischermeier et al. *Angewandte Chemie* 129 (2017) 1289.

I-10

BIOHYDROMETALLURGICAL CONCEPTS FOR METAL RECOVERY FROM PRIMARY AND SECONDARY RESOURCES

K. Pollmann[1,*]

[1]*Helmholtz-Zentrum Dresden-Rossendorf, Helmholtz Institute Freiberg for Resource Technology, D-09599 Freiberg, Germany*

corresponding author: *k.pollmann@hzdr.de*

Keywords: Biohydrometallurgy, bioleaching, biosorption, bioflotation

Novel environmental-friendly technologies are required in order to secure the demand of industrial relevant metals. Such technologies cover the fields of exploitation, beneficiation and recycling of rare elements.

Nature itself offers promising approaches in these fields. In our group we develop bio-based technologies for extracting, treating and recycling critical metals using microbes, microbial metabolites or biomolecules. The presentation gives an overview of current research activities that are performed in our team.

Natural processes such as microbial weathering, biomineralization, or biosorption are highly attractive for biotechnological applications that intend the recovery of metals from primary and secondary resources [1].

Currently applied bioleaching concepts use acidophilic bacteria such as *Acidithiobacillus ferrooxidans* for the extraction of metals from sulfidic ores. This approach is already used for the extraction of copper especially in ores with low metal content. Other concepts use metabolic products from microorganisms for indirect bioleaching processes. For example, in our group we investigate the use of heterotrophic bacteria for the extraction of strategic relevant elements from mining residues.

Biosorption uses the metal binding capabilities of biomass or biomolecules for the recovery of metals from solutions. Such compounds can be immobilized on materials to construct metal selective filter materials. These materials enable an efficient removal of specific metals, and can be regenerated.

Bioflotation introduces particle or ion binding cells or biomolecules in classical flotation procedures for the separation of particles from particle mixtures or metal ions from complex solutions. Biomolecules can replace toxic chemicals.

In conclusion, in combination with established physical and chemical processes, such biotechnological approaches have a high potential to improve metal beneficiation and recycling and contribute to environmentally friendly and sustainable processes.

[1] K. Pollmann, *Biotechnol. Adv*. **36** (2018) 1048-1062.

I-11

NUMERICAL AND ANALYTICAL CONCEPTS OF REACTIVE TRANSPORT TOWARDS PREDICTION OF CONTAMINANT MIGRATION IN THE SUBSURFACE

C. Fischer[1,*], T. Yuan[1], J. Kulenkampff[1], H. Lippold[1], S. Schymura[1], K. Franke[1], Th. Stumpf[2]

[1]Institute of Resource Ecology, HZDR, Permoserstr. 15, 04318 Leipzig, Germany
[2] Institute of Resource Ecology, HZDR, Bautzner Landstr. 400, 01328 Dresden, Germany

* corresponding author: *c.fischer@hzdr.de*

Keywords: Reactive transport modeling, crystal surface reactivity, dissolution, contaminant migration

In this contribution we present aspects of the numerical and experimental work of the Reactive Transport Department of the Institute of Resource Ecology.

One focus is the transport behavior and migration of contaminants in the subsurface. We quantify diffusive and advective flow pathways in complex porous solids by using positron emission tomography techniques. This allows us to identify heterogeneous and anisotropic flow patterns. We also use tomographic methods to reconstruct pore networks over a wide range of the length scale. Spatial resolution typically starts in the nm range, and fields of view span up to ~10 cm. This covers representative elementary volumes that allow the design of robust digital rock models for vigorous numerical simulation of transport [1]. The analytical flow field datasets are used to validate these numerical results.

The second important aspect of our work is the surface reactivity of solids. We investigate amorphous and crystalline materials of natural and synthetic origin with respect to the reaction kinetics during dissolution reactions and sorption processes of contaminants, e.g. for the application of nuclear waste disposal. The variability of surface reactivity is the critical component that determines the predictive quality of reactive transport models. We present rate maps for sorption [2] and dissolution reactions [3] on solid surfaces that document a range of reaction rates of more than three orders of magnitude for chemically identical materials. We discuss the influence of surface defects on these results and the corresponding development of numerical tools for reactive transport [4, 5].

[1] Yuan, T.; Fischer, C. *Transp Porous Media* **138 (2)** (2021) 245.
[2] Yuan, T.; Schymura, S.; Bollermann, T.; Molodtsov, K.; Chekhonin, P.; Schmidt, M.; Stumpf, T.; Fischer, C. *ES&T* **55 (23)** (2021) 15797.
[3] Fischer, C.; Luttge, A. *PNAS* **115 (5)** (2018) 897.
[4] Fischer, C.; Kurganskaya, I.; Luttge, A. *Appl Geoch.* **91** (2018) 140.
[5] Karimzadeh, L.; Fischer, C. *ACS Earth Space Chem.* **5 (9)** (2021) 2408.

I-12

OPTIMIZING THE FROTH ZONE IN MINERAL FLOTATION AND ADSORPTIVE BUBBLE SEPARATION

S. Heitkam[1,2*], B. Keshavarzi[2], T. Krause[3], M. B. Ansorge-Schumacher[3], K. Schwarzenberger[1], K. Eckert[1,2]

[1]Helmholtz-Zentrum Dresden-Rossendorf, Insitute of Fluid Dynamics, Bautzner Landstraße 400,01328 Dresden,Germany
[2]TU Dresden, Institute of Process Engin. and Environmental Techn., 01062 Dresden, Germany
[3]TU Dresden, Department of Molecular Biotechnology, 01062 Dresden, Germany

* corresponding author: *s.heitkam@hzdr.de*

Keywords: froth flotation, foam fractionation, sorption measurement, foam properties

Froth flotation is an important separation processes for the recovery of hydrophobized, valuable minerals from ground ore suspensions. Similarly, adsorptive bubble separation is used to recover surface active materials such as proteins or algae from aqueous solutions. Gas bubbles are introduced to the suspension, picking up the valuable material and transporting it to the top of the container. There, a froth is formed that can be skimmed off to separate the material in high purity.

Key parameter to this process are the froth stability and froth drainage. High froth stability and low drainage will result in extraction of large quantities of the suspension, reducing the purity of the product. Also, froth stability may disturb the downstream processing. But, low froth stability will result in strong drop-back of valuable material and may destroy the process completely.

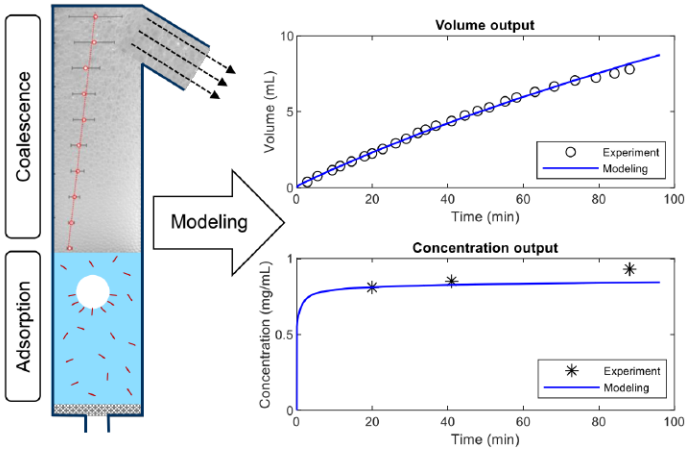


Fig. 1: Sketch of adsorptive bubble separation (left) and resulting volume and concentration output (right).

We combine different measurement techniques to research the amount of adsorbed material on rising bubbles, the froth stability as well as drainage and material flows. Based on these information, we model the overall extraction process and compare our findings to the measured extractions of surface active material and liquid [1]. Additionally, we research and model the process improvement by the addition of wash water to the froth zone.

[1] Keshavarzi, B., Krause, T., Sikandar, S., Schwarzenberger, K., Eckert, K., Ansorge-Schumacher, M. B., & Heitkam, S. *Chem. Eng. Sci.*, **256** (2022) 117715.

Acknowledgements: This work received funding by the German Research Foundation (DFG)under grant numbers HE7529/2-1, HE7529/3-1 and AN 387/7

I-13

SIMULATION OF HYDROGEN SPECIES DIFFUSION BETWEEN LAYERS OF 2D MATERIALS

A. Kuc[1,*]

[1]*Helmholtz-Zentrum Dresden-Rossendorf, Abteilung Ressourcenökologie, Forschungsstelle Leipzig, Permoserstr. 15, 04318 Leipzig, Germany*

* corresponding author: *a.kuc@hzdr.de*

Keywords: metadynamics simulations, hydrogen diffusion, 2D materials

Recent experiments by Geim's group have demonstrated transport and separation of hydrogen isotopes through the van der Waals gap in hexagonal boron nitride (*h*-BN) and molybdenum disulfide (MoS_2) bulk layered materials. The experiments could not distinguish whether the transported particles are protons (H^+) or protium (H) atoms. In one of our recent works, we reported theoretical studies, which indicate that protium atoms, rather than protons, are transported through the gap [1]. First-principles calculations combined with well-tempered metadynamics simulations at finite temperature reveal that for *h*-BN and MoS_2, the diffusion mechanism of both protons and protium (H) atoms involves a hopping process between adjacent layers (see Fig. 1). This process is assisted by low-energy phonon shear modes. The extracted diffusion coefficient of protium matches the experiment, while for protons, it is several orders of magnitude smaller. This indicates that H atoms are responsible for the experimental observations. These results allow for a comprehensive interpretation of experimental results on the transport of H isotopes through van der Waals gaps and can help identify other materials for hydrogen isotope separation applications.

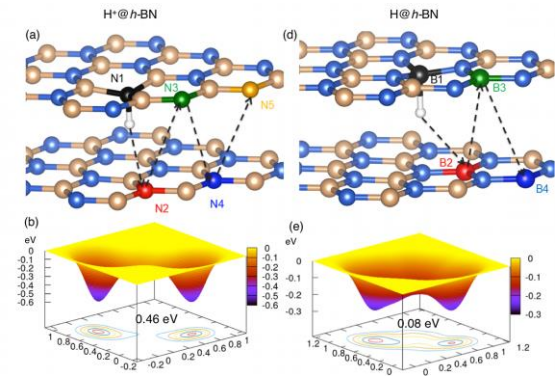


Fig. 1. Well-tempered metadynamics results for H^+ (a, b) and H atom (d, e) simulations between layers of h-BN. (b, e) Free energy profiles for both simulations. Zigzag transport is obtained for both species with very different free energy values.

In more recent investigations, we focus on H atom diffusion between layers of transition-metal dichalcogenides (TMDCs), such as MoS_2, where we investigate the impact of transition metal atom, chalcogen atom, stacking order, and moiré pattern on the diffusion coefficients. We want to learn whether the free energy barriers are lowered (resulting in higher diffusion coefficients) and whether the moiré patterns can enforce directional transport.

We use well-tempered metadynamics simulations in our studies as implemented in the cp2k code. Our approach to H atom diffusion can be extended to investigations of other species, such as Eu(III)-species diffusion in clay mineral layered materials.

[1] Y. An, A. Kuc, P. Petkov, M. Lozada-Hidalgo, T. Heine, *Small* **1901722** (2019) 1-7.

I-14

MATERIALS RESEARCH AT THE DRESDEN HIGH MAGNETIC FIELD LABORATORY

J. Wosnitza*

Hochfeld-Magnetlabor Dresden (HLD), HZDR, 01328 Dresden, Germany

* corresponding author: *j.wosnitza@hzdr.de*

Keywords: materials research, high magnetic fields

In this talk, I will present a brief overview on the experimental infrastructure and the in-house research at the Dresden High Magnetic Field Laboratory (*Hochfeld-Magnetlabor Dresden*, HLD). High magnetic fields are one of the most powerful tools available to scientists for the study, modification, and control of the state of matter. The application of magnetic fields, therefore, has become a commonly used instrument in condensed-matter physics and the demand for the highest possible magnetic-field strengths increases continuously. At the HLD, that has opened its doors for external users in 2007, offers pulsed magnetic fields up to the 90 T range. In the pulsed magnets, a variety of experimental methods are available allowing to measure, for instance, electrical transport, magnetization, magnetostriction, ultrasound, ESR, and even NMR with very high resolution. As a unique feature, a free-electron-laser facility next door (ELBE facility) allows high-brilliance radiation to be fed into the pulsed-field cells of the HLD, thus making possible high-field magneto-optical experiments in the range from 3 to 250 μm. In-house research of the HLD focuses on electronic properties of strongly correlated materials at high magnetic fields. This includes the investigation of novel frustrated magnetic materials and the determination of Fermi surfaces of topological and correlated metals by means of measurements of magnetic quantum oscillations. We further investigate unconventional high-magnetic-field states of novel superconductors, but also field-induced plasma waves in liquid metals – the latter in cooperation with another HZDR institute.

I-15

CENTRE FOR SIMULATIONS OF SUPERDENSE FLUIDS

P. Huovinen[1,*]

[1]*Incubator of Scientific Excellence—Centre for Simulations of Superdense Fluids, University of Wroclaw, Pl. M. Borna 9, 50-204 Wroclaw, Poland*

* corresponding author: *pasi.huovinen@uwr.edu.pl*

Keywords: quark-gluon plasma, heavy-ion collisions

In extremely hot and dense circumstances matter no longer constitutes of atoms, not even protons and neutrons, but of their consituents: quarks and gluons. On Earth this so-called quark-gluon plasma can be formed for a fleeting moment in ultrarelativistic collisions of heavy nuclei, i.e. heavy ions.

Centre for Simulations of Superdense Matter is a newly establised research group in the University of Wroclaw dedicated to modeling these heavy-ion collisions using fluid-dynamical models. In this talk I briefly review the physics of heavy-ion collisions and the research done in the Centre.

I-16

EXPERIMENTAL NUCLEAR ASTROPHYSICS AT FELSENKELLER UNDERGROUND LABORATORY

D. Bemmerer[1,2,*], K. Zuber[2]

[1]*Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstr. 400, 01328 Dresden, Germany*
[2]*Technische Universität Dresden, Zellescher Weg 19, 01062 Dresden, Germany*

* corresponding author: *d.bemmerer@hzdr.de*

Keywords: Nuclear astrophysics, cosmology

The Felsenkeller underground laboratory for experimental nuclear astrophysics includes a 5 MV Pelletron accelerator and Germany's lowest background high-purity germanium detector setup for radioactivity measurements. The laboratory is jointly operated by HZDR and TU Dresden. Due to its 45 m thick rock overburden, in Felsenkeller the cosmic-ray muon flux is 40 times lower than at surface [1], the natural neutron background even 180 times lower [2], and the background in a γ-ray detector with muon veto more than 1000 times lower than at surface [3], enabling highly sensitive nuclear experiments.

The scientific program at Felsenkeller includes the study of astrophysically relevant nuclear reactions. Reactions studied address solar fusion, cosmology, and nucleosynthesis in neutron star precursors.

In addition to reviewing recent progress at Felsenkeller laboratory, the new EU project ChETEC-INFRA [4] will be presented. This EU-funded initiative networks the European research infrastructures for nuclear astrophysics and may also help improve networking between Dresden and Wroclaw specifically.

[1] F. Ludwig et al., *Astropart. Phys.* **112** (2019).
[2] M. Grieger et al., *Phys. Rev. D* (2020).
[3] T. Szücs et al., *Eur. Phys. J. A* (2015).
[4] www.chetec-infra.eu

I-17

EARLY UNIVERSE EVOLUTION FROM LOOP QUANTUM COSMOLOGY

T. Pawłowski [1,*]

[1]*Institute for Theoretical Physics, Faculty of Physics and Astronomy, University of Wrocław, pl. Maksa Borna 9, Wrocław, 50-204, Poland*

* corresponding author: *tomasz.pawlowski@uwr.edu.pl*

Keywords: quantum gravity, quantum cosmology, quantum black holes

Two of the main pillars of modern theoretical physics are General Relativity (GR), accurately describing physical reality in large (astronomical) scales and strong gravitational fields and Quantum Physics (QP, which include quantum mechanics and quantum field theory), describing the reality in microscale. However, these two theories are based on mutually exclusive principles. On the other hand, certain epochs in our Universe history as well as present astrophysical processes require taking into account both the (general) relativistic and the quantum nature of reality. These are, the early Universe and black holes. Their description require a unification of GR and QP – a theory of quantum gravity.

One of most known approaches to such unification is known as Loop Quantum Gravity (LQG). There, the spacetime itself is a quantum object and its geometry is represented by quantum observables. A strict implementation of basic principles of GR resulted in a discrete spacetime structure, where i.e. areas and volumes have discrete spectra. However, due to its level of complication making concrete physical prediction is an enormous technical challenge, which forces one to rely on its simplifications and reductions.

One of such is Loop Quantum Cosmology (LQC), which applies the techniques and some physical input from LQG to cosmological models. There, probing the Universe evolution has changed the big bang paradigm, replacing the initial spacetime singularity with a bounce of prior large (semi)classical contracting universe. Further application of its extensions to black hole description has led to replacing the black hole singularities with the quantum bounce leading to black hole to white hole transition.

Our present is the extension of the physical predictions of LQC to include more realistic physical scenarios. This is being done by extending the existing LQC formalism and by using a slight reduction of the full LQG, simplifying some of its internal mathematical structure. The methodology of probing of the dynamics within these frameworks is based on two components: numerical computation of the quantum state evolution on the genuine quantum level and applying the semiclassical description originating from the Hamburger decomposition. The latter, being applicable to general quantum mechanical systems, allows to encode the quantum state evolution up to arbitrary order (and precision) in a set of (semi) classical equations of motion for specific observables. While it still requires use of high efficiency numerical computing, it is much more efficient than computation of genuine quantum evolution.

Acknowledgements: Work supported in part by the Polish Narodowe Centrum Nauki (NCN) grant 2020/37/B/ST2/03604.

I-18

THEORY OF NONEQUILIBRIUM PHENOMENA

R. Schützhold[1,2,*]

[1]*Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstrasse 400, 01328 Dresden, Germany*
[2]*Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany*

* corresponding author: *r.schuetzhold@hzdr.de*

Keywords: theoretical physics, non-equlilibrium phenomena

This talk will provide a brief introduction into the research activities pursued by the Department of Theoretical Physics at the Helmholtz-Zentrum Dresden-Rossendorf.

I-19

NEUTRINO PHYSICS AND MONTE CARLO SIMULATIONS

J. T. Sobczyk[1,*]

[1]*Institute of Theoretical Physics, University of Wroclaw, plac Maxa Borna 9, Wroclaw, 50-043, Poland*

* corresponding author: *jan.sobczyk@uwr.edu.pl*

Keywords: neutrino, neutrino oscillations, Monte Carlo methods

I will make a case for the significance of neutrino physics and in particular of neutrino oscillation experiments. Their main goal is to check if CP symmetry (C - matter/antimatter symmetry; P - mirror reflection) is broken on elementary level in weak interactions [1]. Results may help us to understand matter/antimatter asymmetry in the Universe. Another goal of neutrino experiments is to search for physics effects beyond the Standard Model.

A new generation of neutrino oscillation experiments (HyperKamiokande in Japan and DUNE in USA) will require substantial reduction of systematic uncertainties including the one coming from a lack of sufficient precision in modeling neutrino interactions [2].

I will describe a contribution from the Wrocław group to this area of research. The most important achievement is development of the Monte Carlo neutrino event generator NuWro which is used worldwide in experimental and theoretical studies [3,4]. A critical part of Monte Carlo generators are modules describing hadron reinteractions in nuclear matter [3,5].

[1] K. Abe, J.T. Sobczyk, The T2K Collaboration, *Nature* **580** (2020) 339-344.
[2] L. Alvares-Ruso, J.T. Sobczyk, …, *Prog. Part. Nucl. Phys.* **100** (2018) 1-68.
[3] T. Golan, C. Juszczak, J.T. Sobczyk, *Phys. Rev. C* **86** (2012) 015505.
[4] Xianguo Lu, J.T. Sobczyk, *Phys. Rev. C* **99** (2019) 055504.
[5] S. Dytman, Y. Hayato, R. Raboanary, J.T. Sobczyk, J. Tena Vidal, N. Vololoniaina, *Phys. Rev. D* **104** (2021) 053006.

I-20

MODIFICATION OF OPTOELECTRONIC PROPERTIES OF TMDC MONOLAYERS BY ION IMPLANTATION

S. Prucnal*

Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, P.O. Box 510119, 01314 Dresden, Germany

* corresponding author: *s.prucnal@hzdr.de*

Keywords: TMDCs, ion implantation, doping, photoluminescence

The efficient integration of 2D materials, like graphene, transition metal dichalcogenides (TMDs) and h-BN into the current electronic device technology requires mastering the techniques of effective tuning of their optical, electronic and magnetic properties. It is crucial to understand how we can tune their conductivity (e.g. n-type or p-type doping), induced ferromagnetism, or valley polarization. For the conventional bulk semiconductors, ion implantation is the most developed method to do this.

In this work, we have investigated the optical and structural properties of different TMDCs modified by ion implantation. We have demonstrated the applicability of ion implantation and post-implantation non-equilibrium thermal processing for tuning the carrier concentration in 2D materials. We demonstrate p-type and n-type doping in TMDCs flakes (starting with 1 ML) realized by low-energy ion implantation of P^+ and Cl^+ ions through a thin capping layer followed by millisecond-range flash lamp annealing (FLA). We further show that FLA for 3 ms is enough to recrystallize implanted $MoSe_2$ and remove ion induced defects.

The comparison between the density functional theory calculations and experimental temperature-dependent micro-Raman spectroscopy data indicates that Cl atoms are incorporated into the atomic network of $MoSe_2$ as substitutional donor impurities. Our results clearly indicate that using our experimental approach, the conventional ion implanters can easily be used to modify the optical, electronic and magnetic properties of various 2D materials on demand.

I-21

ELBE: AN ACCELERATOR DRIVEN RADIATION SOURCE AT ITS BEST

J. M. Klopf[1], A. Arnold[1], P. Evtushenko[1], M. Freitag[1], M. Justus[1], I. Kösterke[1], M. Kuntzsch[1], U. Lehnert[1], A. Ryzhov[1], A. Schamlott[1], C. Schneider[1], R. Schurig[1], A. Schwarz[1], R. Steinbrück[1], R. Xiang[1], K. Zenker[1], P. Michel[1,*]

[1]ELBE Center for High-Power Radiation Sources, Institute for Radiation Physics, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Bautzner Landstraße 400, Dresden, 01328, Germany

* corresponding author: *p.michel@ hzdr.de*

Keywords: accelerator, linac. SRF, FEL, THz, IR, positrons, neutrons, gamma radiation

The heart of the ELBE Center for High Power Radiation Sources is a superconducting RF (SRF) linac, which accelerates electrons up to 35 MeV for driving a diverse set of secondary radiation sources. The ELBE linac is particularly unique in the capability of accelerating a continuous beam of ultrashort bunches of electrons at very high repetition rates (up to 26 MHz). This extremely high-power electron beam is selectively directed into specially designed beamlines to drive secondary radiation sources for THz/IR photons (FELBE and TELBE), positrons (pELBE), neutrons (nELBE), and gamma radiation (γELBE), each with dedicated laboratories and instrumentation. Users from all over the world utilize the advanced radiation sources at ELBE for a wide array of both fundamental and applied studies of matter, health, energy, and technology.

The ELBE accelerator was first commissioned in 2001 in the form of a grid-pulsed 250 kV thermionic gun followed by two stages of RF bunching to inject beam into a linac comprised of two SRF cryomodules, each containing two 9-cell DESY TTF-type niobium accelerating cavities.

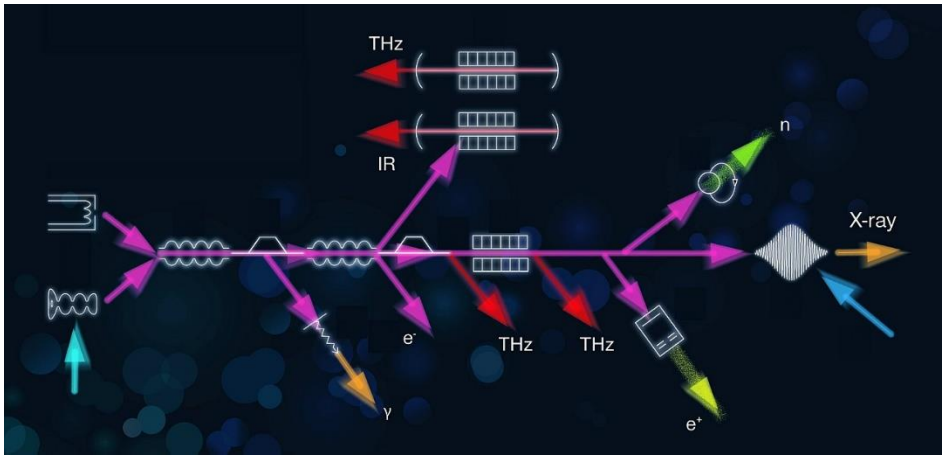


Fig. 1: Schematic of the ELBE linac and secondary radiation sources.

Through continuous development and research, the ELBE facility has achieved many major advancements in accelerator technology, the most important being the ELBE SRF Gun program,

which has designed, built, and commissioned several prototype SRF electron guns for high bunch charge, high average current, and low emittance. The ELBE SRF Gun-II is the first and only electron source of its type to deliver electron beam to a user experiment, and is now in routine operation for the TELBE and pELBE beamlines.

An overview of the performance parameters of the ELBE accelerator and secondary sources will be presented in this talk along with a summary of the experimental capabilities available to users. Highlights of recent user results will also be presented to help illustrate the great potential ELBE provides for a diverse scientific community. Beamtime proposals are accepted and reviewed by an external scientific advisory committee twice per year.

https://www.hzdr.de/db/Cms?pNid=1732

I-22

MATERIALS SCIENCE WITH ION BEAMS AT THE HZDR's ION BEAM CENTER

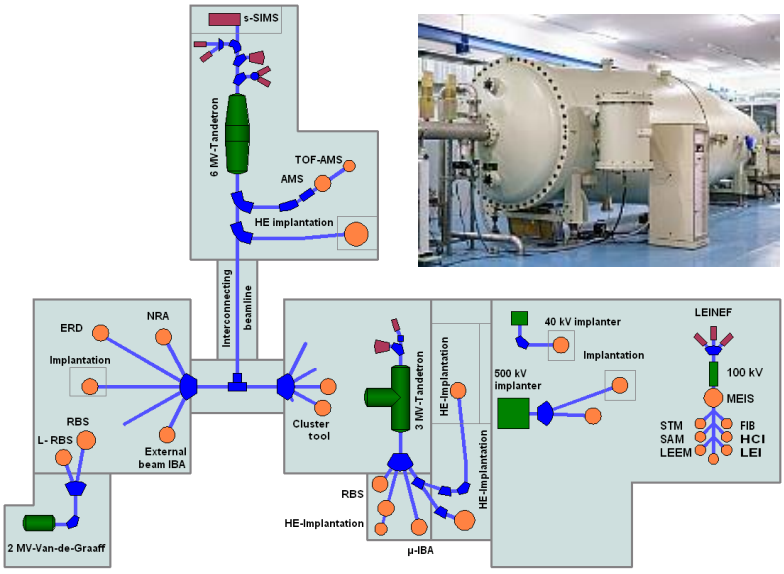
Sh. Akhmadaliev*

Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstr. 400, D-01328 Dresden, Germany

* corresponding author: *akhmadaliev@hzdr.de*

Keywords: ion accelerator, ion implantation, ion beam analysis, accelerator mass spectrometry, focused ion beam, helium ion microscope

The Ion Beam Center (IBC) at the Helmholtz-Zentrum Dresden-Rossendorf (HZDR) is a unique user facility with decades of experience in materials research using ion beams of nearly all stable elements in a wide energy range from some eV up to 60 MeV. The IBC operates several electrostatic ion accelerators, ion implanters, low energy and fine focused ion beam systems (FIB) including helium ion microscope (HIM). The IBC provides experimental equipment for materials modification via ion implantation and irradiation, ion beam analysis of solid and liquid samples, surface processing by low energy and highly charged ions and focused ion beams, as well as measurements at accelerator mass spectrometer (AMS) and a secondary ion spectrometer (SIMS) in combination with the tandem accelerator. Annually, the IBC offers more than 17.000 hours of beam time for research and industrial purposes to users across the globe. Continuous access to the IBC is provided via an online proposal procedure [1] and via transnational access of the Horizon 2020 project RADIATE coordinated by IBC [2].



Additionally, the IBC provides numerous add-on services like sample preparation, clean-room processing, surface and thin film metrology, optical and electron-beam lithography, thermal processing, thin-film deposition, optical and electrical characterization, electron microscopy and spectroscopy, simulation of ion induced processes and data evaluation.

Fig. 1. An overview of ion accelerators at IBC and a photo of 6MV tandem accelerator.

[1] https://www.hzdr.de/db/Cms?pNid=3249
[2] https://www.ionbeamcenters.eu/radiate/radiate-transnational-access/

I-23

IMPROVEMENTS OF THE FINE PARTICLE SEPARATION BY MEANS OF FROTH FLOTATION WITH A SPECIAL FOCUS ON LOCAL POLYMETALLIC RESOURCES

M. Rudolph*, L. Pereira, D. H. Hoang, E. Schach, M. Buchmann, H. Wu, G. van den Boogaart

Helmholtz Institute Freiberg for Resource Technology, Helmholtz-Zentrum Dresden-Rossendorf, Chemnitzer Str. 40, Freiberg, 09599, Germany

* corresponding author: *m.rudolph@hzdr.de*

Keywords: Froth Flotation, Mineral Processing, Cassiterite, Fine Particles, Process Engineering

Fig. 1. Lab Batch Flotation in the labs of Helmholtz Institute Freiberg ©HZDR/Frank Schinski.

This presentation will report on the conclusive findings of various projects revolving around the reprocessing of historic mine tailings in the Erzgebirge region (mountain range in south east Germany bordering Czechia) but also the processing of fresh ore for new exploration projects on polymetallic deposits including the important and partially critical metals: tin, zinc, tungsten, indium, lithium, et al [1, 2]. The main focus will be on innovations in the field of fine particle separation by means of the heterocoagulation process of froth flotation. We will be discussing the use of an additional oily phase to improve the separation as well as the chances and limits of applying microbubbles. Most investigations are making use of quite unique particle characterization and data evaluation approaches which rely on automated mineralogical investigations [2, 3]. Further will we be focusing especially on cassiterite flotation including fundamental investigations applying enhanced atomic force microscopy based methods [4].

The presentation will finally provide an outlook on recent and forthcoming projects which will focus on increasing the level of digitalization and enhancing especially the pneumatic flotation technologies. This will also highlight some already existing and possible future collaborations between Germany and Poland.

[1] T. Leistner et al., *Min. Eng*. **96-97** (2016) 94. | [2] E. Schach et al., *Min. Eng*. **137** (2019) 78. [3] L. Pereira et al. *Min. Eng.* **170** (2021) 107054. | [4] H. Wu et al., *ACS Omega*, **6** (2021) 4212.

Acknowledgements: Thanks for technical support in the experiments to Klaus Graebe and Anja Oestreich and to all the Masters' students working on the BMBF r3 SMSB and BMBF r4 AFK projects

I-24

BUBBLES, SURFACTANTS, PARTICLES: FLUID DYNAMICS ASPECTS OF RESOURCE TECHNOLOGIES

M. Eftekhari[1], A.Bashkatov[1,2], K.Schwarzenberger[1,2], S. Heitkam[1,2], X. Yang[1,2], S. Hossain[1], G. Mutschke[1], K. Eckert[1,2*]

[1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Fluid Dynamics, k.eckert@hzdr.de
Bautner Landstrasse 400, D-01328 Dresden, Germany,
[2]TU Dresden, Institute of Process Engineering and Environmental Technology,
kerstin.eckert@tu-dresden.de, D-01062 Dresden, Germany

* corresponding author: *k.eckert@hzdr.de*

Keywords: bubbles, particles, resource technology, hydrogen

Ressource technologies used e.g. to extract valuable ore particles from gangue mineral, or to produce hydrogen via electrolysis, do heavily rely on multi-phase flows, such as a three-phase flow in the case of flotation or a two-phase flow in the case of electrolyzers. Both flow types are of high relevance in industry and full of fascinating fluid dynamics aspects. In the talk we discuss two of such aspects: the flow on the surface of particle-laden bubbles [1,2] and that on growing hydrogen bubbles [3] at microelectrodes.

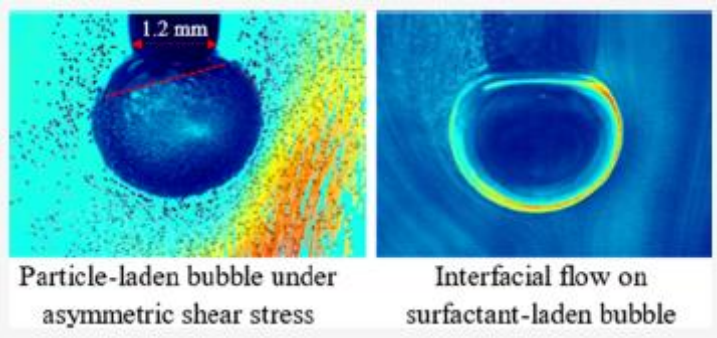


Fig. 2. Micro-Particle Image Velocimetry pictures showing the flow on the surface of air bubbles driven by an asymmetric shear flow; taken from [1].

[1] M. Eftekhari, K. Schwarzenberger, S. Heitkam, A. Javadi, A. Bashkatov, S. Ata, K. Eckert, *Langmuir* **37** (2021), 13244.
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[3] A. Bashkatov, S. Hossain, X. Yang, G. Mutschke, K. Eckert, *Phys. Rev. Lett.* **123** (2019), 214503

I-25

DALI - HZDR NEXT-GENERATION IR-THz, VUV PHOTON SOURCE FOR ULTRAFAST SCIENCE

P. Evtushenko[1,*], J.-C. Deinert[1], J. M. Klopf[1], S. Kovalev[1]

[1]Bautzner Landstrasse 400, Dresden, 01328, Germany

* corresponding author: *p.evtushenko@hzdr.de*

Keywords: THz, High-field, VUV, FEL, SRF LINAC, accelerator-based

The ELBE radiation source operated by HZDR is a user facility based on a 1 mA, 40 MeV CW SRF LINAC. The user facility includes several MIR and THz sources: two FEL oscillators and one coherent undulator source. The sources are operated with pulse energies on the order of a few μJ and with a repetition rate of 13 MHz in the case of the FEL oscillators and 100 kHz in the case of the coherent undulator source. The latter is operated simultaneously with a single-cycle, broadband THz source based on coherent diffraction radiation (CDR) with a pulse energy of a few 100 nJ. We have proposed to construct a new accelerator-based ELBE-successor user facility DALI (Dresden Advanced Light Infrastructure). The main point of the new facility would be to increase the MIR-THz pulse energy by 2 to 3 orders of magnitude. The new facility would include new MIR-THz, sources with pulse energies in the range from 100 μJ to about 1 mJ, operating at the high repetition rates between 100 kHz and 1 MHz in the frequency range from 0.1 to 30 THz with a bandwidth of a few percent. The new THz facility would also include single-cycle THz sources, with an electrical field strength of a few MV/cm. In this contribution, we outline key aspects of a new radiation source concept, which would allow achieving such parameters. Another part of the proposed facility would be a CW VUV FEL operating in the wavelength range from 50 through 250 nm with a high repetition rate matching the repetition rate of the high-energy IR-THz sources. The VUV FEL would operate with the pulse energy on the order of 30 μJ and a pulse length of 100 fs. Presently this wavelength range is not covered by any fully coherent, high repetition rate, ultrafast photon source. A short overview of the key design idea of the VUV FEL will be also presented.

The main motivation for the new facility construction is its scientific case. The new MIR-THz sources would enable new, presently not available, experimental regimes for nonlinear THz photonics [1], nonlinear plasmonic [2], spintronics [3], and Floquet engineering [4]. The VUV FEL will enable transformative changes in physical chemistry research, specifically for gas- and liquid-phase chemistry and heterogeneous catalysis, and will move us closer to the fundamental understanding of mechanisms of chemical reactions.

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I-26

CHALLENGES IN THE SYNTHESIS OF NANOMATERIALS WITH REQUIRED PROPERTIES

M. Buryi*

FZU – Institute of Physics of the Czech Academy of Sciences, Cukrovarnická 10/112, Prague, Czechia

* corresponding author: buryi@fzu.cz

There is a wide spectrum of human activities, existing and emerging, where optical materials are implemented. This can be light emitting diodes, polarizers, photodetectors, scintillators etc. The scintillators occupy the special niche in the everyday human life. These are the transformers/detectors of the high energy incident radiation. They find implementation in many aspects of the scientific, industrial, environmental, societal and health development. The most demanding are the fields of medicine and homeland security, including the monitoring of radiation leakages (e.g., at nuclear power plants or nuclear waste disposals). As an example of medical application, the positron emission tomography (PET) or computed tomography (CT) could be given. There, the gamma rays and X-rays are detected, respectively. In both cases, the increased sensitivity and timing characteristics of the scintillating detector would result in the decreased dose of the irradiation delivered to the living tissues and/or organs of a patient. Good candidates are zinc oxide (ZnO), gallium nitride (GaN) and cesium lead bromide ($CsPbBr_3$, CPB) having great potential to be implemented in the time-of-flight (TOF) applications as well. By moving from the bulk three-dimensional (3D) single crystals to the nanoscale materials (wires (1D), thin films, e.g., (multiple) quantum wells ((M)QW, 2D) and quantum dots (0D)) the rise of the efficiency of the radiation detector is observed.

ZnO has excellent physical properties. It is cheap and can be easily grown as a nanopowder, in the form of free-standing nanorods or nanorods deposited onto a substrate.

GaN has scintillating properties very similar to those of the ZnO. It can be synthesized in the variety of forms as well. One of the forms is indium doped GaN (InGaN) MQW grown on a GaN layer – a kind of thin film multilayer structure, where the thickness of a single layer is about 2-3 nm. These exhibit good scintillating properties.

CPB grown as larger nanoparticles or quantum dots has prominent timing characteristics, large light and quantum yields.

However, there are several drawbacks. (i) ZnO is ageing, and its scintillation properties suffer from defects and charge trapping centers. Moderation of the growth conditions and/or post-growth treatment as well as the injection of dopants can solve this problem, at least, partly. (ii) GaN structures suffer from accidental carbon and zinc impurities entering the GaN and InGaN hosts from precursors. These can partly be compensated by doping GaN with Si or Ge. (iii) CPB is hygroscopic, and, therefore, the ways of avoiding it coming to the contact with vapour from air should be established. These are the main challenges faced by the material scientists all over the world. By addressing them, the abilities of the mentioned nanomaterial scintillators can be pushed to the theoretically predicted limits. This is the the aim of the present research.

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I-27

PERSPECTIVES OF DIGITAL CHEMISTRY

T. Heine[1,2,*]

[1]*Helmholtz Center Dresden-Rossendorf, Leipzig Research Branch, Permoserstr. 15, 04318 Leipzig, Germany*
[2]*Technische Universität Dresden, Mommsenstr. 13, 01062 Dresden, Germany*

* corresponding author: *t.heine@hzdr.de*

Keywords: Digital Chemistry, Artificial Intelligence, Chemputation, Research Data Management in Chemistry

Data science and artificial intelligence are entering the field of chemistry and have the potential to revolutionize it. For example, the reproducibility of chemical reactions has been an issue for decades if not centuries (despite clear instructions), and modern research data management combined with automated synthesis approaches are likely to overcome this issue.

TU Dresden and FAU Erlangen-Nuremberg are preparing a proposal for the next German Excellence Initiative where Digital Chemistry is a central aspect. In my presentation, I will highlight the cornerstones or our initiative and will discuss potential overlap with CASUS. The presentation shall provide the basis for further discussions during CASUSCON and afterwards.

I-28

MULTIVARIATE INTERPOLATION IN NON-TENSORIAL NODES LIFTS THE CURSE OF DIMENSIONALITY FOR TREFETHEN FUNCTIONS

M. Hecht[1,*]

[1]*Center for Advanced Systems Understanding (CASUS), Untermarkt 20, 02826 Görlitz, Germany*

* corresponding author: *m.hecht@hzdr.de*

Keywords: interpolation, curse of dimensionality

1D Polynomial interpolation goes back to Newton, Lagrange, and others and its fundamental importance in mathematics and computing is undisputed. We extended Newton and Lagrange interpolation to arbitrary dimensions while maintaining their numerical stability and computational efficiency. Our generalization relies on a proper choice of non-tensorial *unisolvent interpolation nodes* whose number scales sub-exponentially with the space dimension. The resulting interpolation scheme is proven to approximate all functions of the largest Hilbert space of Sobolev functions that is contained in the space of continuous functions. We further demonstrate that the resulting polynomial interpolant empirically reaches the optimal exponential approximation rate for the Runge function, suggesting its optimality for a class of functions we term *Trefethen functions*. Combining sub-exponential node counts with exponential approximation rates, the proposed non-tensorial choice of unisolvent nodes may *lift the curse of dimensionality* for interpolation problems of Trefethen functions.

I-29

EXCITATION OF AN INHOMOGENEOUS ELECTRONIC SYSTEM: FROM AMBIENT CONDITIONS TO WARM DENSE MATTER

Z. Moldabekov*

CASUS, Helmholtz-Zentrum Dresden-Rossendorf

* corresponding author: z.moldabekov@hzdr.de

Warm dense matter (WDM) is the state of matter at high pressures and temperatures. WDM is relevant both for practical applications and for fundamental science. The practical significance is due to the generation of the WDM state in experiments on nuclear fusion and the creation of new materials under extreme conditions. From the point of view of fundamental science, the relevance of WDM is due to the extreme conditions in the interiors of planets and stars.

Many questions regarding the interplay of quantum degeneracy, thermal excitations, and strong correlations effects in WDM remain open. To solve this problem, we use an externally perturbed WDM to investigate how electronic structure and excitations are affected by thermal excitations and density inhomogeneities. The results are reported in our recent articles [1-4], where we presented: a study of the quality of various exchange-correlation functionals in the KS-DFT method [1,2]; the change in electronic excitations due to strong inhomogeneity and thermal effects [3]; and a new KS-DFT based methodology for the investigation of the non-linear response of electrons across temperature regimes relevant for WDM [4].

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I-30

SELF-CORRECTING QUANTUM MANY-BODY CONTROL USING REINFORCEMENT LEARNING WITH TENSOR NETWORKS

M. Bukov[1,*]

[1]*Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, 01187, Dresden*

* corresponding author: *mgbukov@pks.mpg.de*

Quantum many-body control is a central milestone en route to harnessing quantum technologies. However, the exponential growth of the Hilbert space dimension with the number of qubits makes it challenging to classically simulate quantum many-body systems and consequently, to devise reliable and robust optimal control protocols. I will present a novel framework for efficiently controlling quantum many-body systems based on reinforcement learning (RL). We tackle the quantum control problem by leveraging matrix product states (i) for representing the many-body state and, (ii) as part of the trainable machine learning architecture for our RL agent. The framework is applied to prepare ground states of the quantum Ising chain, including critical states. It allows us to control systems far larger than neural-network-only architectures permit, while retaining the advantages of deep learning algorithms, such as generalizability and trainable robustness to noise. In particular, I will demonstrate that RL agents are capable of finding universal controls, of learning how to optimally steer previously unseen many-body states, and of adapting control protocols on the fly when the quantum dynamics are subject to stochastic perturbations.

I-31

PROTON THERAPY: TODAY AND IN THE FUTURE

C. Richter*

Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstrasse 400, 01328 Dresden, Germany

* corresponding author: *c.richter@hzdr.de*

Abstract not provided.

I-32

CAR-T CELLS IN PEDIATRIC PATIENTS WITH LEUKEMIA AND SOLID TUMORS. CURRENT STATUS AND FUTURE PERSPECTIVES

K. Kalwak*

Wroclaw Medical University, Department of Pediatric Bone Marrow Transplantation, Oncology and Hematology, Borowska 213 St. 50-556 Wroclaw, Poland

corresponding author: *krzysztof.kalwak@umw.edu.pl*

Keywords: CAR-T cells, immunotherapy, leukemia, solid tumors

The most famous 'proof' in favor of CD19-targeted chimeric antigen receptor T (CAR-T) cell therapy is Emily Whitehead, the first child to have her own immune cells trained to fight cancer. It worked, and Emily has been cancer-free now for more than ten years. CAR-T cell therapy is a groundbreaking treatment that has launched a new era in the treatment of hematological malignancies. Safety and efficacy evaluation of tisagenlecleucel (Kymriah®) in children was conducted in a clinical trial, ELIANA and in 2017, Kymriah® became the first CAR-T cell therapy approved by the US Food and Drug Administration (FDA) for patients aged up to 25 years who suffer from B-cell precursor acute lymphoblastic leukemia that is refractory or in a second or subsequent relapse. In 2018, tisagenlecleucel was also approved by the European Commission. CAR-T cell technology is an excellent example of cell gene therapy that is highly personalized to target an individual patient's disease. To create CAR-T cells, a patient's own T lymphocytes need ex vivo genetic manipulation. A gene encoding CAR anti-CD19 is introduced into the genome of T cell with the help of lentiviral vectors. After activation and expansion, ready-to-use CAR-T cells are obtained. When infused into the bloodstream, CAR-T cells are able to penetrate tissues, self-activate, amplify, eliminate neoplastic cells, and act long-term. The first Polish patient was successfully treated with CAR-T cell therapy in November 2019 at the Department of Hematology and Transplantology in Poznan. He was a 24-year-old male with refractory, early relapsed diffuse large B-cell lymphoma (DLBCL) after autologous stem cell transplantation. Also in November 2019, our center was approved by Novartis to become the first pediatric certified site for CAR-T cell therapy in Poland. The first implementation was performed in March 2020 in an 11-year-old boy with multiply relapsed acute lymphoblastic leukemia. Now, after more than 28 months post infusion, the patient remains disease-free and requires immunoglobulin substitution due to most welcome prolonged B-cell aplasia. But it is not the end: our center aims at developing advanced therapies based on cells, genes and small molecules. It all starts in a research lab - none of the advanced therapies can be created without preclinical research. Close cooperation of clinicians and scientists, and the exchange of research observations from two different perspectives (laboratory vs. patient) ensure the constant development of medicine. The results of research from scientific laboratories can be directly used to develop new ways of treating patients and the treatment is tailored to the molecular needs of the patient Our research task remains development of an innovative CAR receptor and production of CAR-T cells "in house" and designing individual receptor domains. To our target diseases belong: T-cell ALL, AML, and solid tumors incl. neuroblastoma or glioma.

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I-33

WHY META-RESEARCH IS IMPORTANT AND CAN WE MAKE IT MORE EFFICIENT

B. Helfer[1,2*]

[1]*Meta Research Centre, University of Wrocław, ul. K. Szajnochy 7/9, Wrocław, 50-438, Poland*
[2]*Institute of Psychology, University of Wrocław, ul. Dawida 1, Wrocław, 50-529, Poland*

* corresponding author: *bartosz.helfer@uwr.edu.pl*

Keywords: meta-research, evidence synthesis, risk of bias, data science

Meta-Research Centre at the University of Wroclaw aims to improve the mechanism of science by monitoring its transparency, rigour and biases, synthetizing evidence and perfecting research methods, so scientific results can be better, faster, more usable and precise.

Meta-research ("research on research") is the best approach for understanding whole fields of research and correcting their course [1]. Meta-research investigates methods and practices to reduce bias and enhance reliability of scientific studies. It encompasses evidence synthesis and evaluation of credibility and trustworthiness of research findings with the goal of increasing value (e.g. by fostering research integrity, transparency, replicability and independence) and reducing waste by improving research practice [2].

There is a crisis of reproducibility, integrity and transparency looming large across clinical sciences [3]. It has been estimated that as much as 85% of resources invested go to waste due to wrong incentives, leading to multiple biases, such that most negative results are never reported and more than 50% of published studies are reported selectively [4]. In anonymous surveys, a clear majority of scientists admit using questionable research practices to achieve more attractive results [5]. A growing consensus of scientific opinion questions the transparency and integrity of industry sponsored clinical trial practices [6]. Meta-research is considered the best approach to help solve precisely such a crisis [7].

However, to achieve such lofty goals, meta-research, including its various branches, should become more efficient and robust itself. This requires constant and creative introduction of best available methods for harvesting large, good quality datasets and analysing them. How to consistently achieve that remains unclear, but undoubtedly developing a successful approach requires an interdisciplinary effort spanning data science, systems theory, machine learning and natural language processing.

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I-34

NUMERICAL MODELS OF THE HUMAN BRAIN

M. Ptak[1,*]

[1]*Wroclaw University of Science and Technology, Wyb. Wyspianskiego 27, 50-370 Wroclaw, Poland*

* corresponding author: *mariusz.ptak@pwr.edu.pl*

Keywords: brain, finite element analysis, impact, biomechanics

Detection of the pathomechanism of the destruction of brain structures is critical in terms of prevention and treatment [1]. The main goal of the aHEAD project is the continuous improvement of diagnostic methods and simulations of the influence of impact on the brain structure, reflecting the consequences of road accidents, sport injuries and improving head protection devices, including ski, bicycle and motorcycle helmets. Due to the cooperation with neurosurgeons and neurobiologists, the project team gained extensive knowledge about the properties of the structure of the brain structures, and through experimental studies, we obtained precise input data for numerical models of the human head. The research involved medical imaging processing, advanced material processing, biomechanics, computer science and neurosurgery inputs – the fields which are often considered separately. Finally, we created a set of state-of-the-art models for a small child, middle-aged and a senior person (Fig. 1). In addition, we made publicly available an educational system that allows access to a simplified human head model to visualize the effects of stress on the structure of the brain [2]. The system allows verifying the level of load on the head of a small child in order to check the shaken baby syndrome on a generalized model. Additionally, we constructed a multi-sensor headband for recording mechanical loads on the human head in real-time, including electroencephalography. After a proper validation process, it is now possible to perform a numerical simulation of the structural destruction of brain tissues under mechanical loading at the tissue-level in two different numeric codes: LS-DYNA and Abaqus.

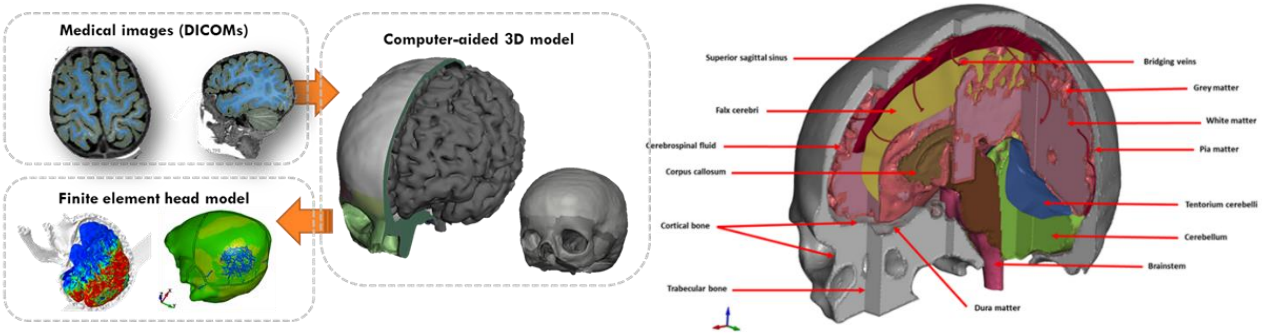

Fig. 3. Modelling at the tissue level – the stages of modelling of a human head (left) and a section of a numerical model for middle age person in LS-DYNA (right).

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I-35

SOME THEORETICAL ASPECTS OF REPROGRAMMING THE STANDARD GENETIC CODE

P. Błażej*

Faculty of Biotechnology, University of Wroclaw,
ul. F. Joliot-Curie 14a, 50-383 Wroclaw, Poland

* corresponding author: *pawel.blazej@uwr.edu.pl*

Abstract not provided.

I-36

REGULARIZATION TECHNIQUES IN THE ANALYSIS OF LARGE DATA SETS

M. Bogdan[1,*]

[1]*Uniwersytet Wrocławski, Malgorzata.Bogdan@uwr.edu.pl, Wroclaw, 50-137, Poland*

** corresponding author: malgorzata.bogdan@uwr.edu.pl*

Keywords: statistics, dimensionality reduction, large data sets

High-dimensional data is currently ubiquitous in many areas of science and industry. Acquiring a knowledge from such data sets is hindered by the curse of dimensionality, which leads to increased variance of statistical estimators, large numbers of false discoveries and the loss of power of identifying important relations. Regularization methods stabilize the variance of statistical estimators by applying penalties on the statistical model complexity. In this talk we will briefly recall the idea of regularization and discuss several classical and modern approaches to this problem. We will mainly concentrate on the LASSO and SLOPE penalties, which induce the dimensionality reduction and allow to identify the low-dimensional structures behind the data generation process. The talk will be illustrated with computer simulations and the real data examples from medicine, genetics and finance.

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I-37

DATA-DRIVEN AND PHYSICS-INFORMED MODELING OF MATTER UNDER EXTREME CONDITIONS

A.Cangi [1,2,*]

[1]*Center for Advanced Systems Understanding, Untermarkt 20, 02826 Görlitz, Germany*
[2]*Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany*

* corresponding author: *a.cangi@hzdr.de*

Keywords: Materials Science, Electronic Structure, Machine Learning, Neural Networks

The successful characterization of high energy density (HED) phenomena in laboratories using pulsed power facilities and coherent light sources is possible only with numerical modeling for design, diagnostic development, and data interpretation. The persistence of electron correlation in HED matter is one of the greatest challenges for accurate numerical modeling and has hitherto impeded our ability to model HED phenomena across multiple length and time scales at sufficient accuracy. Standard methods from electronic structure theory capture electron correlation at high accuracy, but are limited to small scales due to their high computational cost. In this talk I will summarize our recent efforts on devising a data-driven and physics-informed workflow to tackle this challenge. Artificial intelligence (AI) has great potential for accelerating electronic structure calculations to hitherto unattainable scales [1]. I will present our recent efforts on speeding up Kohn-Sham density functional theory calculations with deep neural networks in terms of our Materials Learning Algorithms framework [2,3]. Similarly, our results on automated machine-learning save orders of magnitude in computational cost for finding suitable neural networks [4]. Furthermore, our surrogates both predict the electronic structure, its dynamics, and yield thermo-magneto-elastic materials properties of matter under extreme conditions highly efficiently while maintaining their accuracy [5,6]. Finally, I will conclude with a preview on our most recent result that enables neural-network-driven electronic structure calculations for systems containing more than 100,000 atoms.

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I-38

CORRELATIONS IN DENSE MATTER

G. Röpke*

Institute of Physics, University of Rostock, D-18051 Rostock, Germany

* corresponding author: *gerd.roepke@uni-rostock.de*

Keywords: Nuclear matter equation of state, Symmetry energy, Supernova explosions, Ionization potential depression, Electrical conductivity of dense plasmas, Pauli blocking, Mott effect

The properties of hot and dense matter are of interest not only in astrophysics, but also in laboratory physics, materials science, energetics, and other fields. Correlations, especially the formation of bound states, determine these properties. Many-particle theories are applied to nuclear matter and electron-ion plasmas. Green's functions and numerical simulations are used to calculate thermodynamic and transport properties in dense fermion systems.

The composition of nuclear matter under supernova conditions and heavy ion collisions is discussed [1]. Different approaches to the treatment of bound state formation, continuum correlations, and in-medium effects are presented [2]. An in-medium Schroedinger equation is derived and the formation of quantum condensates is shown.

The degree of ionization and transport properties of plasmas under extreme conditions are studied [3,4]. Path-integral Monte-Carlo and DFT-molecular dynamics simulations are compared with analytical results [5]. The properties of warm and dense matter are of interest for planetary physics but also for laboratory experiments with high-intensity short-pulse laser irradiation.

The formation of bound states, quasiparticle shifts, screening, Pauli blocking, quantum condensates, and the Mott effect are interesting phenomena that govern the physical properties of hot and dense matter.

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I-39

INSIGHTS OF QCD PHASE STRUCTURE FROM HADRON SPECTROSCOPY AND RESONANCE GAS MODEL

P. M. Lo[1,*], K. Redlich[1]

[1]*University of Wroclaw, pl. Uniwersytecki 1, Wroclaw, 50-137, Poland*

* corresponding author: *pokman.lo@uwr.edu.pl*

Keywords: hadron resonance gas, QCD phase diagram, scattering, LQCD

Heavy ion collision (HIC) experiment is entering the era of precision. The new generations of high statistics and precision experiments shall unravel detailed structure of matter, giving us the opportunity to disentangle multiple competing mechanisms contributing to observables. At the same time there are significant improvement in the precision of thermal lattice QCD (LQCD) results on the fluctuations of combinations of conserved charges in the confined phase. To properly interpret these data and make progress in relating them to the underlying dynamics it is necessary to refine our existing theoretical analysis tools.

A very detailed picture of hadronic interactions emerged from an impressive volume of scattering experiment data, and extensive theoretical studies such as chiral perturbation theory and LQCD. We shall discuss how the statistical hadronization model, improved with a scattering matrix (S-matrix) formulation of statistical mechanics, provides the necessary framework to make direct use of this resources for investigating the phenomenology of heavy ion collisions.
As an application we will present an analysis on proton and Lambda yields from the heavy ion collision experiments at the LHC. We will discuss how inconsistencies between theory and experiment, e.g. the proton puzzle and the proton to Lambda ratio, may be resolved by considering some essential features of the empirical baryon spectrum. These dynamical features are also crucial for understanding the Lattice results on thermal QCD, such as the baryon electric charge correlation.

I-40

MATTER UNDER EXTREME CONDITIONS IN NEUTRON STARS AND THEIR MERGERS

D. Blaschke[1,*], O. Ivanytskyi[1], T. Fischer[1], A. Bauswein[2]

[1]Institute of Theoretical Physics, University of Wrocław, 50-204 Wrocław, Poland
[2]GSI Helmholtzzentrum für Schwerionenforschung GmbH, D-64291 Darmstadt, Germany

* corresponding author: *david.blaschke@uwr.edu.pl*

Keywords: Density functional, quark matter deconfinement, neutron star mergers, supernova explosions

We outline the role that an early deconfinement phase transition from normal nuclear matter to a color superconducting quark-gluon plasma phase plays for the phenomenology of supernova explosions and binary neutron star mergers. To this end we develop a density functional approach to the equation of state (EoS) of quark matter with confinement and color superconductivity [1] and construct the transition to the EoS of the hadronic matter phase from vanishing to moderately high temperatures that will become accessible also in future terrestrial experiments with heavy-ion collisions. For the first time a phase transition construction is developed that allows for multiple critical points in the QCD phase diagram, including the possibility of a "crossover all over" [2].
We study the connection of such hybrid EoS with the mass-radius relation of cold compact stars, including the intriguing possibility of additional families, as a consequence of the presence of an early and strong phase transition. Special emphasis is devoted to the simultaneous fulfillment of the new constraint from the NICER mass and radius measurement on PSR J0740+6620 and the tidal deformability constraint from the binary neutron star merger event GW170817 which require the EoS to be soft at about twice saturation density and to stiffen at higher densities. Such a pattern is provided by an early and strong deconfinement transition [1]. We discuss whether the deconfinement signals remain intact which have recently been found in dynamical astrophysical scenarios, such as binary compact star mergers including the subsequent emission of gravitational waves [3] and supernova explosions of massive supergiant stars where neutrinos and gravitational waves play the role of messengers [4,5].

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I-41

OBSERVABILITY OF COULOMB-ASSISTED QUANTUM VACUUM BIREFRINGENCE

N. Ahmadiniaz[1,*], M. Bussmann[2,1], T. E. Cowan[1,3], A. Debus[1], T. Klug[1], R. Schuetzhold[1,4]

[1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstrasse 400, Dresden, 01328, Germany
[2]Center for Advanced Systems Understanding (CASUS), Goerlitz, 02826, Germany
[3]Institut fuer Kern-und Teilchenphysik, Technische Universitaet Dresden, 01062, Germany
[4]Institut fuer Theoretische Physik, Technische Universitaet Dresden, 01062, Germany

* corresponding author: *n.ahmadiniaz@hzdr.de*

Keywords: Vacuum birefringence, Coulomb potential, XFEL .

We consider the scattering of an x-ray free-electron (XFEL) beam on the superposition of a strong magnetic field $\mathbf{B}_{\mathbf{ext}}$ with the Coulomb field $\mathbf{E}_{\mathbf{ext}}$ of a nucleus with charge number Z. In contrast to Delbrueck scattering (Coulomb field only), the magnetic field $\mathbf{B}_{\mathbf{ext}}$ introduces an asymmetry (i.e., polarization dependence) and renders the effective interaction volume quite large, while the nuclear Coulomb field facilitates a significant momentum transfer $\Delta\mathbf{k}$. For a field strength $\mathbf{B}_{\mathbf{ext}}=10^6$ T (corresponding to an intensity of order 10^{22} W/cm^2) and an XFEL frequency of 24 keV, we find a differential cross section $d\sigma/d\Omega \sim 10^{-25}\, Z^2/(\Delta\mathbf{k})^2$ in forward direction for one nucleus. Thus, this effect might be observable in the near future at facilities such as the Helmholtz International Beamline for Extreme Fields (HIBEF) at the European XFEL [1].

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I-42

QUANTUM DYNAMICS FAR FROM EQUILIBRIUM

M. Kaminski[1,2,*]

[1]*Department of Physics and Astronomy, University of Alabama, 514 University Boulevard, Tuscaloosa, AL 35487, USA*
[2]*on sabbatical leave at Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany*
v
* corresponding author: *mski@ua.edu*

Keywords: quantum many-body, thermalization, gauge/gravity correspondence, entanglement

A quantum computer stores information in a large number of interacting quantum bits, qubits. These qubits need to be written and read fast and careful enough, because they come with an "expiration date". This is caused by a quantum mechanical effect called "decoherence". This constitutes a fundamental open problem, namely to understand and control the dynamics of rapidly changing quantum many body systems, i.e. systems far away from being in equilibrium. Remarkably, we can experimentally generate such states of matter in heavy-ion-collisions for example at the Relativistic Heavy Ion Collider at Brookhaven National Laboratory, Upton, NY, at the Large Hadron Collider, CERN, Geneva, Switzerland, as well as in a very different setting, within ultra-cold atom gases, or we may observe these effects in astrophysical black holes or neutron stars [1]. Universal underlying concepts are the same, although, of course, the energy range, temperature and many other parameters are vastly different. Focusing on the common features of these distinct systems will lead us to the discovery of the essential fundamental principles that govern quantum dynamics far from equilibrium and the evolution of quantum information as well as entanglement [2]. This constitutes a powerful fundamentally novel approach to problems in quantum computing, leveraging the wealth of knowledge, methods and experiments from particle and gravitational physics [3, 4, 5].

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I-43

FRONTIERS OF COMPUTATIONAL QUANTUM MANY-BODY THEORY

T. Dornheim[1,2,*]

[1]*Center for Advanced Systems Understanding (CASUS), Görlitz, Germany*
[2]*Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany*

* corresponding author: *t.dornheim@hzdr.de*

Keywords: Computational physics, quantum chemistry, warm dense matter, high-performance computing

The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved." Nearly a century has passed, yet the famous quote by Paul Dirac still gets to the heart of many research fields within theoretical physics, quantum chemistry, material science, etc. In this talk, I will show how we can use cutting-edge numerical methods on modern high-performance computing systems to effectively overcome these limitations in many cases. In this way, we get unprecedented insights into quantum many-body systems on the nanoscale going all the way from ultracold atoms like superfluid helium to warm dense matter that occurs within planetary interiors and thermonuclear fusion applications.

I-44

TUNING MAGNETIC PROPERTIES BY INTRODUCING DEFECTS

K. Potzger[1,*], S. Anwar[1,2], and R. Bali[1]

[1]*Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstrasse 400, 01328 Dresden, Germany*
[2]*Technische Universität Dresden, 01062 Dresden, Germany*

* corresponding author: *k.potzger@hzdr.de*

Keywords: magnetic thin films, ion irradiation, defects

In certain binary alloys such as $Fe_{60}V_{40}$, B2 $Fe_{60}Al_{40}$ [1], B2 $Fe_{50}Rh_{50}$ [2], the saturation magnetization (Ms) can be tuned by inducing structural disorder by means of energetic ion-irradiation. Here we present the magneto-structural phase transition in all three materials with respect to static and dynamic magnetic properties. Under Ne^+ ion irradiation in the keV energy range, $Fe_{60}V_{40}$ transforms from the structurally short-range ordered phase of the as-grown film to the A2-phase accompanied by a drastic increase of Ms up to ~750 kA/m. The ferromagnetic phase shows a low damping parameter of 0.0027 ± 0.0001. Under similar irradiation conditions, paramagnetic B2 $Fe_{60}Al_{40}$ transforms into the ferromagnetic A2 phase with Ms up to ~710 kA/m. Local ion irradiation can be used for nanoscale magnetic patterning. For Ne^+ irradiation of $Fe_{50}Rh_{50}$ thin films, the transition temperature of the metamagnetic phase transition, from the antiferromagnetic to the ferromagnetic phase, shifts from 370 K towards lower temperatures. At the same time, a ferromagnetic background develops which dominates the magnetic properties after irradiation at large ion fluencies. The change of the magnetic properties is discussed with respect to static structural disorder.

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Acknowledgements:Funding by the Deutsche Forschungsgemeinschaft (DFG) – 322462997 (BA 5656/1-2 | WE 2623/14-2) is acknowledged.

I-45

SPACE AND SATELLITE RESEARCH AT UPWr

K. Sośnica*, W. Rohm, T. Hadaś, J. Kapłon, K. Kaźmierski, M. Ilieva, R. Zajdel, G. Bury

Wrocław University of Environmental and Life Sciences, Leading Research Gr, Grunwaldzka 53, Wrocław, 50-357, Poland

* corresponding author: *krzysztof.sosnica@upwr.edu.pl*

Satellite techniques are very extensively used for monitoring the Earth system, including the natural environment, changes induced by climate change and anthropogenic activities. This contribution summarizes the scientific activities related to space and satellite research conducted at the Institute of Geodesy and Geoinformatics of the Wroclaw University of Environmental and Life Sciences (UPWr).

In the framework of the European Plate Observing System for Poland (EPOS-PL), UPWr has developed a monitoring system of anthropogenic Earth surface and building deformations in the mining and post-mining areas with the implementation in the Upper Silesia region. The monitoring system incorporates ground-based and satellite observations to provide comprehensive information on the land subsidence and seismicity using classical surveying methods, remote sensing, as well as gravimeters and receivers of Global Navigation Satellite Systems (GNSS). The surface monitoring is based on satellite interferometric synthetic aperture radars (InSAR) supported by GNSS and levelling measurements for accuracy assessment and validation. Moreover, UPWr participates in the international consortia and projects, e.g., in the European Space Agency's project "Fundamental techniques, models and algorithms for a Lunar Radio Navigation system (ATLAS)" that aims at developing a satellite navigation system for the Moon. Scientists at UPWr developed a model for satellite orbit perturbations that allows for the precise orbit determination of Earth's artificial satellites and other celestial bodies, including the Moon. The orbit model includes all gravitational and non-gravitation orbit perturbations as well as major and secondary effects emerging from general relativity to accurately determine and predict the position of spacecraft. UPWr specializes also in the modelling of the microwave and laser signal delays in the Earth's atmosphere. The most recent achievements and results of developing satellite techniques used for Earth monitoring and modelling of environmental processes observed from satellites will be discussed during the presentation.

I-46

DISCRETE OPTIMIZATION IN THE ERA OF QUANTUM COMPUTING - A CASE STUDY

W. Bożejko

Department of Control Systems and Mechatronics,
Faculty of Information and Communication Technology
Wroclaw University of Science and Technology,
Wyb. Wyspianskiego 27, 50-370 Wroclaw, Poland

* corresponding author: *wojciech.bozejko@pwr.edu.pl*

Keywords: quantum annealing, discrete optimization, scheduling, NP-hard problem

Quantum computers are slowly becoming a tool for effectively solving difficult optimization and decision-making problems. Although this process is progressing slowly, the computing power of modern quantum machines (comparable to classical computers in the 1950s-60s of the previous century) is growing rapidly, and in some areas even exceeds the capabilities of supercomputers. In particular, solving problems of the NP-hard class, for which solving methods with polynomial computational complexity on classical computers are unknown so far, is a challenge. The very design of an algorithm solving an optimization problem with a non-trivial objective function, e.g. total weighted tardiness, using a quantum machine is a challenge in itself. This is due to the fact that the way a problem is prepared for a quantum machine is subject to many limitations.

The quality of the obtained results is a separate problem. Apart from the probabilistic nature of this type of calculations and the lack of repeatability of the results, another issue is the optimality of the obtained result. Nevertheless, it turns out that it is possible to obtain some strong results in this field, i.e. to show that a quantum computer is able to generate optimal results, despite the fact that as a device (considering e.g. D-Wave quantum machines using hardware quantum annealing) it performs kind of heuristics.

I-47

HUMAN AND ANIMAL MOBILITY - INTEGRATED SCIENCE OF MOVEMENT AT UPWr SpaceOs

W. Rohm[1,*], K. Smolak[1], V. Brum-Bastos[1,2], B. Hordyniec[1], K. Siła-Nowicka[1,3], K. Knop[4], M. Łoś[1]

[1]Wrocław University of Environmental and Life Sciences, Leading Research Gr, Grunwaldzka 53, Wrocław, 50-357, Poland
[2]University of Canterbury, School of Earth and Environment, Private Bag 4800, Christchurch, 8140, New Zealand
[3]University of Auckland, School of Environment, Science Center 301, 23 Symonds St, Auckland, 1010, New Zealand
[4]U+GEO Sp z o.o., Grunwaldzka 53/127, Wrocław, 50-357, Poland

* corresponding author: witold.rohm@upwr.edu.pl

Keywords: human mobility, movement ecology, integrated science of movement, big data

Movement is studied across a number of disciplines ranging from GIScience, movement ecology, geography, transportation, public health to computer science, and physics. It is usually studied either as individual (Lagrangian) or population-based (Eulerian) movement.
The first is referred to as the movement of individuals (human or animal) across space and time and it is producing trajectories, while the former is concerned with flows or presence of individuals or groups in space and time. Both types are important to both human mobility (e.g. four steps model in transportation), and movement ecology (e.g. wild bird migration routes).
Following [1] and [2] integrated science of movement is currently being developed that is providing a framework for understanding human and animal movement in both Lagragian and Eulerian perspectives.
SpaceOs Leading Research Group of UPWr is approaching the movement analytics from numerous perspectives: in a collective flow modeling efforts with 4W (WHO - WHERE – WHEN - WEATHER) model [3], individual trajectories analytics with HuMobi library [4], human mobility modeling in disease spread prediction on the individual level [5], animal behawior studies based on the trajectory analytics [6], as well as applications in human domain – utility demand forecasting [7].
This crossdisciplinarity of research in both human mobility and movement ecology is gradually breaking the barriers between major research fields.

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I-48

ANIMAL MOVEMENT RESEARCH AS A CROSS-CUTTING THEME AT CASUS

J. Calabrese*

CASUS - Center for Advanced Systems Understanding, Helmholtz-Zentrum Dresden-Rossendorf e.V. (HZDR), Untermarkt 20, 02826 Görlitz

* corresponding author: *j.calabrese@hzdr.de*

Abstract not provided.

I-49

AIR POLLUTION AND ALLERGENIC POLLEN - INTEGRATED APPROACH TO MODELLING, MEASUREMENTS & HEALTH EFFECTS

M. Werner*, M. Kryza, A. Drzeniecka-Osiadacz, T. Sawiński, M. Malkiewicz

Faculty of Earth Sciences and Environmental Management, University of Wrocław, Wrocław, Cybulskiego 30, 50-205, Poland

* corresponding author: *malgorzata.werner@uwr.edu.pl*

Keywords: air pollution, modelling, monitoring, allergenic pollen

We aim to present the system of atmospheric processes modelling and monitoring which is operating at the University of Wroclaw. The system is an integrated tool, optimized for the analysis of the processes taking place in the atmospheric boundary layer, with a particular emphasis on the air pollution and allergenic pollen concentrations. State-of-the-art atmospheric chemical transport models are used to provide air pollution forecasts and made available for a wide community on a website https://prognozy.uni.wroc.pl/. The forecasting system is constantly developed to provide the best possible quality of temporal and spatial distribution of air pollution concentrations. Modelling at a very high spatial resolution of tens of meters, modelling of allergenic pollen or data assimilation of surface and satellite observations are the most urgent research tasks currently undertaken.

The monitoring system of meteorological and air pollution parameters covers measurements with stationary and mobile equipment (sensors mounted on a drone or car). An unmanned aerial vehicle (drone) is equipped with an environmental head that measure air pollution concentrations (e.g. particulate matters, ozone) and meteorological parameters such as air temperature, humidity and atmospheric pressure. Another important part of the monitoring system is remote-sensing measurements by means of a sodar and this year lidar, sun and lunar photometers will be installed (Wrocław is a member of Actris network). This year an automatic, real-time allergenic pollen monitor will contribute to resources of our unit. The site will be the best equipped air quality and pollen monitoring site in Poland.

The results of recently undertaken research as well as future plans in the area of atmospheric processes modelling and monitoring will be presented and discussed.

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I-50

TITLE NOT PROVIED

M. Nikl*

Institute of Physics, Academy of Sciences of The Czech Republic,
Cukrovarnicka 10, 162 00 Prague 6, Czech Republic

* corresponding author: *nikl@fzu.cz*

Abstract not provided.

I-51

DATA-DRIVEN DESIGN OF TWO-DIMENSIONAL NON-VAN DER WAALS MATERIALS

R. Friedrich[1,*], M. Ghorbani-Asl[1], S. Curtarolo[2], A. V. Krasheninnikov[1]

[1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, Dresden, 01328, Germany
[2]Duke University, 144 Hudson Hall, Durham, NC 27708, United States

* corresponding author: *r.friedrich@hzdr.de*

Keywords: data-driven materials design, 2D materials, exfoliation

Two-dimensional (2D) materials are traditionally associated with the sheets forming bulk layered compounds bonded by weak van der Waals (vdW) forces with graphene derived from bulk graphite being the most prominent example. The weak inter-layer interaction leads to a natural structural separation of the 2D subunits in the crystals, giving rise to the possibility of mechanical and liquid-phase exfoliation. The anisotropic interaction also provided suitable structural criteria for the computational search for such traditional 2D materials which predicted about 2000 exfoliable compounds [1].

However, the unexpected experimental realization of atomically thin sheets from non-vdW bonded compounds, for which the previously formulated descriptors are not applicable, recently opened up a new direction in the research on 2D materials [2]. These non-vdW 2D compounds exhibit qualitatively new features due to the unsaturated bonds at their surfaces. Here, we present our recent data-driven search for representatives of this novel materials class [3]. By screening the AFLOW database according to structural prototype information 28 new, potentially synthesizable candidates are outlined. The oxidation state of the surface cations is found to regulate the exfoliation energy with low oxidation numbers giving rise to weak bonding – thus providing an enabling descriptor to obtain novel 2D materials. The candidates showcase a versatile spectrum of appealing electronic, optical and magnetic properties suggesting in particular spintronic applications.

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I-52

SCREENING PROTEOMES FOR PREDICTION AND DESIGN OF ANTIMICROBIAL PEPTIDES WITH AMPGRAM

P. Gagat[1,*], K. Sidorczuk[1], F. Pietluch[1], J. Kała[2], D. Rafacz[2], L. Bąkała[2], J. Słowik[2], R. Kolenda[3], J. Chilimoniuk[1], S. Rödiger[4], L. C. H. W Fingerhut[5], I. R Cooke[5], P. Mackiewicz[1], M. Burdukiewicz[6]

[1]University of Wroclaw, Faculty of Biotechnology, Poland
[2]Warsaw University of Technology, Faculty of Mathematics and Information Science, Poland
[3]Wrocław University of Environmental and Life Sciences, Faculty of Veterinary Medicine, Poland
[4]Brandenburg University of Technology Cottbus-Senftenberg, Faculty of Natural Sciences, Germany
[5]Department of Molecular and Cell Biology, Centre for Tropical Bioinformatics and Molecular Biology, James Cook University, Australia
[6]University of Bialystok, Clinical Research Centre, Poland

* corresponding author: *przemyslaw.gagat@uwr.edu.pl*

Keywords: antimicrobial peptides, benchmarks, machine learning, negative sampling, prediction, reproducibility

Antimicrobial peptides (AMPs) are molecules widespread in all branches of the tree of life. They participate in host defense and/or microbial competition. Due to their positive charge, hydrophobicity and amphipathicity, they preferentially disrupt negatively charged bacterial membranes. AMPs are considered an important alternative to traditional antibiotics, especially at the time of multidrug-resistant bacteria being on the rise. Therefore, to reduce the costs of experimental research, robust computational tools for AMP prediction and identification are essential. AmpGram is our novel tool for AMP prediction that uses n-grams (amino-acid motifs) and random forests (a machine learning method) as an AMP classification algorithm. It is worth emphasizing that an extensive benchmark analysis indicated AmpGram as the most stable and best-performing architecture among top-ranking AMP classifiers. It is also the first AMP prediction tool created for longer AMPs and can be used for high-throughput proteomic screening. Moreover, AmpGram also provides a list of shot 10 amino acid fragments in the antimicrobial regions, along with their probability predictions; these can be used for further studies and the rational design of new AMPs. AmpGram is available as a web-server: http://biongram.biotech.uni.wroc.pl/AmpGram/ and was deposited at GitHub repository: https://github.com/michbur/AmpGram-analysis.

Poster Session

P-1

MODIFIED $Y_3(Al,Ga)_5O_{12}:Pr^{3+}$ AS A DUAL-MODE LUMINESCENCE THERMOMETERS

P. Bolek[1, *], J. Zeler[1], C. D. S. Brites[2], J. Trojan-Piegza[1], L. D. Carlos[2], E. Zych[1]

[1]Faculty of Chemistry, University of Wroclaw
14. F. Joliot-Curie Street, 50-383 Wroclaw, Poland
[2]University of Aveiro, Physics Department, CICECO-Aveiro Institute of Materials
3810-193 Aveiro, Portugal

* corresponding author: *paulina.bolek@uwr.edu.pl*

Keywords: luminescence thermometry, Pr^{3+} luminescence, $Y_3Al_5O_{12}$, bandgap engineering

The precise and accurate measurement of temperature is crucial in many areas, like biomedicine, nanomedicine, electronics, production of plants, aerospace, catalysis, and space research. Luminescence thermometry is of growing interest for such purposes. Being a noninvasive spectroscopic technique based on the phosphor temperature emission dependence (e.g., intensities of luminescence, peak position, lifetime, rise time) it offers important advantages over the presently used remote technics in this field [1] and is nowadays considered the most promising and perspective remote technique of temperature measuring.

In this presentation, we will show the spectroscopic properties of Ga-modified $Y_3Al_5O_{12}$:Pr phosphor and their usefulness in temperature measuring. The studies were performed for the whole family of Ga-modified $Y_3(Al_{1-x},Ga_x)_5O_{12}$:Pr (Ga x=0-1) phosphors. This presentation shows how the Al:Ga ratio in the garnet host lattice affects phonon energies of the host, its refractive index, and bandgap energy and, consequently, how it impacts various aspects of luminescence of the Pr^{3+} activator. We will show important advantages the use of the 5d→4f Pr^{3+} luminescence may offer by utilizing the luminescence intensity ratio as well as luminescence kinetics to measure temperature using these dual-mode luminescence thermometers. Our approach allows obtaining thermometers that work over a range of temperature as broad as 17-700 K and offers the maximum relative sensitivity up to 3.60 $\%K^{-1}$ combined with admirable accuracy, well below 0.05 K [2].

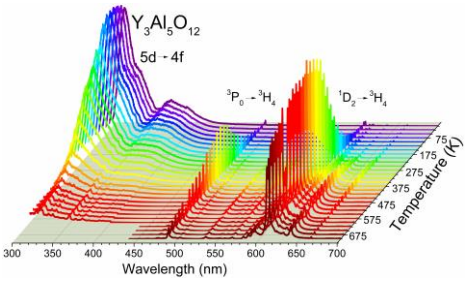

Fig. 1. Emission spectra for $Y_3Al_5O_{12}$:Pr registered under 280 nm excitation at 17-700 K.

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P-2

Mn^{4+} LUMINESCENCE FOR HORTICULTURAL AND LIGHTING APPLICATIONS

J. Jedoń[1,*], A. Lazarowska[2], T. Leśniewski[2], S. Mahlik[2], M.G. Brik[3,4,5], M. Piasecki[5], A.M. Srivastava[6], W.W. Beers[6], and E. Zych[1]

[1]Faculty of Chemistry, University of Wroclaw
14. F. Joliot-Curie Street, 50-383, Wroclaw, Poland
[2]Institute of Experimental Physics, Faculty of Mathematics, Physics and Informatics, University of Gdańsk, Wita Stwosza 57, 80-308 Gdańsk, Poland
[3]College of Sciences & CQUPT-BUL Innovation Institute, Chongqing University of Posts and Telecommunications, Chongqing, 400065, People's Republic of China
[4]Institute of Physics, University of Tartu, W. Ostwald Str. 1, Tartu, 50411, Estonia
[5]Theoretical Physics Department, Jan Dlugosz University, 42-200, Czestochowa, Poland
[6]Current Lighting Solutions, LLC, 1099 Ivanhoe Road, Cleveland, Ohio 44110

* corresponding author: *joanna.jedon@chem.uni.wroc.pl*

Keywords: Mn^{4+} luminescence, horticultural phosphors, pressure sensing, structural disorder

Detailed studies on luminescence of Mn^{4+} in the series of three isostructural double perovskites: $Ba_2LaNbO_6:Mn^{4+}$, $Ba_2La(Zr_{0.5},W_{0.5})O_6:Mn^{4+}$, and $Ba_2La(Nb_{0.8},Zr_{0.1},W_{0.1})O_6:Mn^{4+}$, were performed in the temperature range of 10-500 K as well as at different pressures. Key parameters responsible for both energy and intensity of the $^2E_g \rightarrow {}^4A_{2g}$ zero-phonon emission transition were defined. To further advance the understanding of the observed experimental dependencies, the Mn^{4+} energy levels were calculated using the exchange charge model (ECM) of the crystal-field theory. The correlation between chemically induced structural disorder and the luminescence of Mn^{4+} was found. Broadening of the Mn^{4+} ion luminescent features was observed with increasing cationic sublattice disturbance, (see Fig. 1). The changes observed in experimental data are consistent with the results of the ECM calculations.

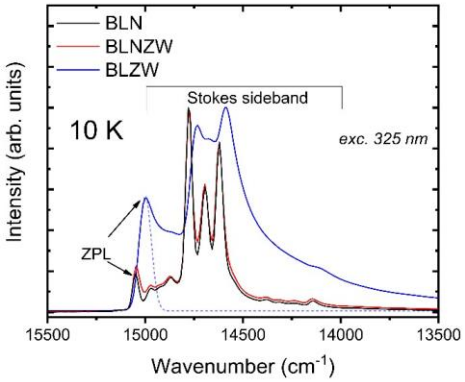

Fig. 1. Low temperature emission spectra of (a) $Ba_2LaNbO_6:Mn^{4+}$ (BLN), (b) $Ba_2La(Nb_{0.8}Zr_{0.1}W_{0.1})O_6:Mn^{4+}$ (BLNZW) and (c) $Ba_2La(Zr_{0.5}W_{0.5})O_6:Mn^{4+}$ (BLZW) in wavenumber scale. The line ca. 15000 cm^{-1} is the zero phonon line (ZPL), while the rest of the lines constitute Stokes phonon sideband. In case of sample (c), the ZPL was reconstructed by Gaussian fit of the edge of the emission spectrum (dashed line), due to overlap between ZPL and phonon structure.

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P-3

MICROBIOTA OF SNAKES FREE-LIVING IN POLAND WITH SPECIAL CONCERN TO *SALMONELLA* SSP.

M. Małaszczuk[1], A. Pawlak[1*], S. Bury[2], A. Wzorek[3], A. Korzeniowska-Kowal[3], M. Cichoń[4], G. Bugla-Płoskońska[1]

[1] Department of Microbiology, Faculty of Biological Sciences, Stanisława Przybyszewskiego 63-77, 51-148 Wrocław, University of Wrocław
[2] Department of Comparative Anatomy, Institute of Zoology and Biomedical Research, Jagiellonian University, Gronostajowa 9, 30-387 Kraków, Poland
[3] Department of Immunology of Infectious Diseases, Hirszfeld Institute of Immunology and Experimental Therapy, Polish Academy of Sciences, Weigla 12, 53-114 Wrocław, Poland
[4] Institute of Environmental Sciences, Jagiellonian University; Gronostajowa 7, 30-387 Kraków

** corresponding author: aleksandra.pawlak@urw.edu.pl*

Keywords: microbiota, reptiles, salmonella, biofilm

Currently, zoonoses, i.e., human diseases caused by contact with an animal (direct or indirect contact), are a global problem of public health. The World Health Organization (WHO) estimates that 60% of all infectious diseases are zoonoses, and millions of people die every year [1]. Zoonoses constitute 75% of all emerging diseases discovered in the last 20 years [2]. The subject of the intestinal microbiota of wild animals in Poland has been little known so far. Most of the studies available in the literature concern *Salmonella* spp. isolated from breeding exotic reptiles and amphibians (most publishes in the PubMed database come from the USA and China), while very little is known about free-living European reptiles and amphibians. The research results obtained by the research team of the Department of Microbiology of the University of Wrocław - describing the intestinal microbiota of grass snake (*Natrix natrix*) free-living in Poland are pioneering [3]. We isolated 19 species of Gram-negative bacteria, and *Salmonella* was third in terms of the frequency of occurrence among the isolates tested. *Salmonella* spp. do not cause any disease symptoms in reptiles, being their natural intestinal flora. Cases of zoonoses have been documented - transmission of *Salmonella* from reptiles to humans and the induction of severe disease symptoms in people at risk, i.e., children under 5 years of age, the elderly, patients with immunological deficiencies, and pregnant women. It is still unclear why reptiles are asymptomatic, but transmission to humans leads to infections, sometimes fatal. One of the factors that can significantly affect the virulence of bacteria is their growth temperature. Reptiles, as animals with the ability to thermoregulate (the optimum body temperature of *N. natrix* is 30°C), undergoing hibernation, during which their body temperature drops significantly, are in this context a completely different host for bacteria than humans. Our results indicates that *Salmonella* spp. is able to form biofilms in the room temperature and 28°C and in our opinion, thanks to this form, do not cause disease symptoms in the host, while at 37°C bacteria become planktonic form and may then be virulent towards the host.

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P-4

INTRACELLULAR NANOTHERMOMETERS IN MAPPING OF CANCER CELLS TEMPERATURE

J. Zeler[1,2,*], R. Piñol[3], C. D. S. Brites[2], Y. Gu[3,4], P. Téllez[5], A. N. Carneiro Neto[2], Th. E. da Silva[2,6], R. Moreno-Loshuertos[7], P. Fernandez-Silva[7], A. Gallego[7], L. Martinez-Lostao[7], A. Martínez[8], L. D. Carlos[2], A. Millán[3]

[1]Faculty of Chemistry, University of Wroclaw, Wroclaw, Poland
[2]CICECO-Aveiro Institute of Materials, University of Aveiro, Aveiro, Portugal
[3]ICMA, Institute of Materials Science of Aragon, CSIC-University of Zaragoza, Zaragoza, Spain
[4]School of Materials Science and Engineering. Nanjing Tech University, Nanjing PR China
[5]Servicio de Apoyo a la Investigación. University of Zaragoza, Zaragoza, Spain
[6]Department of Fundamental Chemistry, Federal University of Pernambuco, Recife, PE, Brazil.
[7]Departamento de Bioquímica, Universidad de Zaragoza, Zaragoza, Spain
[8]Departamento de Electrónica de Potencia, I3A, Universidad de Zaragoza, Zaragoza, Spain

* corresponding author: *justyna.zeler@uwr.edu.pl*

Keywords: intracellular thermometry, polymeric micelles, thermogenesis of the cells

We will present here a unique system for real-time intracellular temperature mapping of living cells based on innovative luminescent Eu^{3+}/Sm^{3+}-bearing polymeric micellar probes. The micelles and the Ln^{3+} complexes covalently bonded to its hydrophobic part were rationally designed to mitigate quenching effects induced by the culture medium. Moreover, the copolymerization strategy proposed permits easy incorporation of other functionalities, such as targeting different cell organelles, and the temperature is recorded from the ratio between the integrated areas of the transitions of the Sm^{3+} and Eu^{3+} ions, respectively, using a conventional fluorescence microscope. A proof-of-concept experiment on breast metastatic adenocarcinoma cells incubated with the Eu^{3+}/Sm^{3+}-bearing micelles under UV-light excitation yields 2D thermal images in the 296–304 K range with an uncertainty of 0.2 K. The thermal images allow us to delimitate the cells and to identify its nucleolus as brighter regions (see Fig.1a). By increasing the temperature of the culture medium, inhomogeneous intracellular temperature progressions up to ~20 degrees and an increment of ~5 degrees of the nucleolus temperature relative to the rest of the cell were discerned, which might be related to the activity of the thermo-generating organelles and highly exoenergetic processes (Fig. 1b).

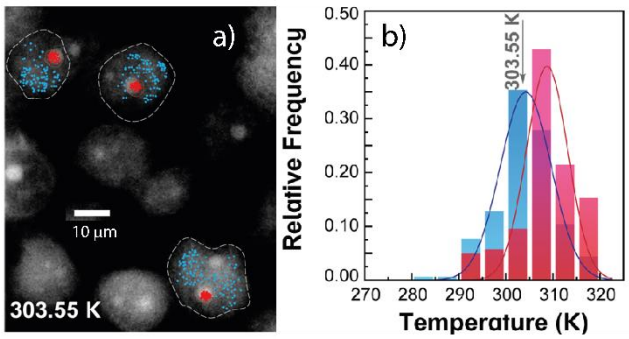

Fig. 4. Microscopy image of the MDA-MB-468 cells incubated with polymeric micelles. The blue and red points mark, respectively, the locations used for temperature determination of the darker and brighter regions (a). On the right (b), temperature histograms obtained from the selected points indicated in the image.

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P-5

DIFFERENTIATION ANTICANCER FROM ANTIMICROBIAL PEPTIDES USING CANCERGRAM

K. Sidorczuk, M. Burdukiewicz, D. Rafacz, F. Pietluch*, M. Bąkała, J. Słowik, P. Gagat

Faculty of Biotechnology, University of Wrocław,
ul. F.Joliot-Curie 14a, Wrocław, 50-383, Poland

* corresponding author: *filip.pietluch2@uwr.edu.pl*

Antimicrobial peptides (AMPs) are a group of biologically active molecules, mainly short peptides from 5 to 100 amino acids. They provide i.e., multicellular organisms with protection against microorganisms. Some AMPs can target cancer cells; therefore, they are called anticancer peptides (ACPs). Due to their small size, hydrophobicity, positive charge, hydrophobicity and amphipathicity, AMPs and ACPs interact with negatively charged components of biological membranes. AMPs preferentially penetrate microbial membranes, but ACPs also target the mitochondrial and plasma membranes of cancer cells. Given the therapeutic potential of ACP and the millions of cancer deaths each year, finding new cationic peptides that selectively destroy cancer cells is critical. ACPs prediction employs a variety of computational approaches; however, there are serious concerns about the quality and quantity of sequences used for its development. As a result, these algorithms have problems distinguishing peptides with similar compositions but different activities, i.e., between AMPs and ACPs. Some do not provide web servers and, thus, have limited use to biologists unfamiliar with bioinformatics. Therefore, to solve this problem and reduce the cost of experimental research, we developed a powerful computational tool, CancerGram, which uses n-grams and random forests to predict ACPs. Compared to other ACP classifiers, CancerGram is the first three-class model that effectively classifies peptides into: ACPs, AMPs and non-ACPs/non-AMPs, with AU1U amounting to 0.89 and a Kappa statistic of 0.65. CancerGram is available as a web server and R package.

P-6

FORCED *SALMONELLA SPP.* LABORATORY ADAPTATION TO DISINFECTANTS IN SUB-LETHAL CONCENTRATIONS LEADS TO RESISTANCE TO ANTIBIOTICS. USAGE OF BIOCIDES PRUDENTLY

B. Futoma-Kołoch*, G. Bugla-Płoskońska

Department of Microbiology, Faculty of Biological Sciences, University of Wrocław, Przybyszewskiego 63-77, bozena.futoma-koloch@uwr.edu.pl, gabriela.bugla-ploskonska@uwr.edu.pl, Wrocław, 51-148, Poland

* corresponding author: *bozena.futoma-koloch@uwr.edu.pl*

Keywords: *Salmonella*, disinfectant, adaptation, cross-resistance

Salmonellosis is the second most common food-borne zoonotic disease in countries of European Economic Area and European Union after campylobacteriosis [1]. *Salmonella* rods are equipped with many virulence factors necessary in the pathogenesis of infections, but of particular interest is their ability to produce biofilms. It is known that microorganisms existing in consortia become less susceptible to chemical elimination due to difficult penetration of antimicrobial agents (AA) including biocides. Biofilms can form on the produced food, in pipes, on the walls, floor, countertops, in places where surfaces meet, various gaps, as well as devices and elements made of materials such as nylon, stainless steel, glass, rubber, aluminum or polystyrene. The best strategy for eliminating bacterial biofilms from food processing environments is to prevent their formation by using materials that will hinder bacterial colonization (more costly), or by using disinfecting procedures or a combination of both. It is worth noting that the effectiveness of a given disinfectant depends on the concentrations of the active substances and the properties of the bacteria themselves [2,3,4]. In laboratory conditions, it has been repeatedly shown that culturing bacteria in the presence of disinfectants and allowing them to gradually adapt to biocides results in tolerance to the AA, but also (as an undesirable side effect) to some classes of antibiotics such as co-trimoxazole, cefotaxime and ciprofloxacin. This dangerous phenomenon, referred to as cross-resistance, may occur when: a) bacteria have formed biofilms, b) when disinfectants are too diluted or c) biocide is not thoroughly rinsed from the cleaned surface [4,5,6]. Work on this issue has been carried out in the Department of Microbiology since 2015. In connection with the above, it is justified to comply with the principles of GHP, GMP and the HACCP system. Proper washing and disinfection especially in industrial plants protect against developing of antimicrobial resistance.

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P-7

GALLERIA MELLONELLA- SMALL LARVAE WITH A HUGE POTENTIAL IN PATHOGENICITY, CYTOTOXICITY AND PHARMACOINENTICS TESTING IN MOLECULAR MICROBIOLOGY

M. Książczyk* , B. Dudek, K. Korzekwa, G. Bugla-Płoskońska

[1] *Department of Microbiology, Faculty of Biological Sciences, University of Wrocław*

* corresponding authors: *marta.ksiazczyk@uwr.edu.pl* , *gabriela.bugla-ploskonska@uwr.edu.pl*

Keywords: pathogenicity, bacteria, alternative in vivo model

The in vivo assays are crucial and are used as a gold standard in a very wide range of scientific trials and projects. However, the application of the laboratory animals has many limitations of ethical, logistical and financial concern. As a result, the researchers began to make other alternative options for experimental animals [1]. Very promising and used with increasing success for several years are insect models. The invertebrates do not have nociceptors so they are insensitive to pain; consequently, there are no restrictive ethical rules unlike for vertebrates [2]. Among the invertebrates, for some time the greatest interest of the family of scientists is the wax moth Galleria mellonella, and more precisely the stage of larvae. There is a broad range of benefits of the application of the wax moth larva. What is the most important, the insect immune system is analogous to the innate mammalian immune response and pathogen killing occurs by similar mechanisms. Moreover the use of the wax moth model is low cost, larvae could be incubated in 37 C and what is important, the accurate inoculum of the pathogen can be delivered directly into the larvae hemocoel. Finally, and crucially, the wax moth model is also amenable for assessing the efficacy of antimicrobial agents, and this model has been used to study therapeutics for infections, cytotoxicity tests and pharmacokinetic tests of therapeutics compounds [3,4,5]. We want to present a broad range of utilization of larvae model in biological sciences.In the Department of Microbiology, we have been using larval tests for several years to study the virulence of Gram-negative bacteria. In our own research we have tested the pathogenicity of uropathogenic E. coli (UPEC) strains. Larvae were injected with the inoculum of each tested bacterial strain prior to washing the bacterial mass in the PBS buffer. As a control, ten larvae were injected with sterile PBS. After injection, larvae were incubated in 37 C for 120 h. The survival of larvae were checked every 24 h. In results we have received one of tested strains presenting a very high pathogenicity (0% of the larvae had survived after injection). We had also assigned the LD50 value.

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P-8

Lu-BASED GARNETS AS THERMOMETRIC PROBES

J. Trojan-Piegza*, J. Zeler, E. Zych

Faculty of Chemistry, University of Wroclaw
14. F. Joliot-Curie Street, 50-383 Wroclaw, Poland

* corresponding author: *joanna.trojan-piegza@uwr.edu.pl*

Keywords: luminescence thermometer, LuAG, temperature-dependent photoluminescence, garnets

Optical sensors are expected to find applications in medical, industrial or military fields. These sensors are used to measure the pressure, radiation, humidity, temperature, and so forth. An example of such sensors are optical thermometers. These sensors measure the object temperature remotely and draw extensive attention nowadays. Their mechanism is based on variation of optical properties as the temperature changes. Among all optical thermometry methods, such as Raman scattering or optical microscopy, luminescence thermometry attracted most attention. Being a fast and simple, this non-contact thermometric method has been the subject of extensive research in recent years.

The concept of luminescence thermometry has been widely applied in lanthanide-doped inorganic materials, metal−organic frameworks (MOFs) and recently in molecular lanthanide compounds. Herein, we present a Pr^{3+}-doped lutetium-based family of garnets as temperature sensors over the 13−700 K range. Possibility of using these phosphors for temperature measurements is studied by analyzing the temperature effects on their photoluminescence spectra and kinetics.

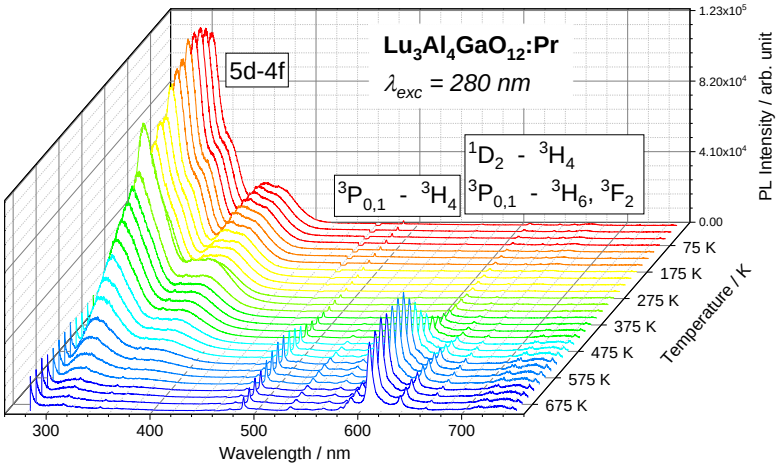

Fig. 5. Temperature dependence of photoluminescence spectra of Pr-doped lutetium aluminium-galium garnet excited with UV radiation.

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P-9

LUMINESCENCE THERMOMETRY USING Pr-ACTIVATED GARNETS

D. Kulesza*, J. Zeler*, P. Bolek, J. Trojan-Piegza, E. Zych, and J. Sadowski

Faculty of Chemistry, University of Wroclaw,
14. F. Joliot-Curie Street, 50-383 Wroclaw, Poland

* corresponding author: *dagmara.kulesza@chem.uni.wroc.pl & justyna.zeler@chem.uni.wroc.pl*

Keywords: luminescence thermometry, garnets, Pr^{3+}-luminescence

Pr-activated garnets are specific phosphors in which the Pr^{3+} ion can be efficiently excited optically by its 4f→5d allowed absorption transition using UV-C radiation and can produce three types of emissions, afterward. Thus, the 5d→4f broadband luminescence in the UV-blue part of the spectrum as well as narrow lines resulting from the $^3P_0 \rightarrow {}^3H_J$ and $^1D_2 \rightarrow {}^3H_4$ transitions in the bluish-green and red part of the spectrum are generated, respectively. The three emissions have much different properties and, consequently, their temperature dependence is diverse. Therefore we considered the Pr^{3+} luminescence very attractive for luminescence thermometry. Since garnets are mostly thermodynamically stable oxides they can withstand drastic changes of temperature from helium to above 1500 °C even. This makes them easy to operate also in quite harsh conditions.

We shall review in detail the possibilities to control complex electronic processes in Pr-activated garnets important for luminescence thermometry. The host lattice–activator interaction will be discussed and conclusions concerning the possibility to design and tune luminescent thermometers for a broad range of temperature sensing will be considered, see Fig. 1. We show that Pr-doped garnets may be attractive luminescence thermometers for measurements at low, intermediate, and high temperatures, which is nowadays a real challenge in this field.

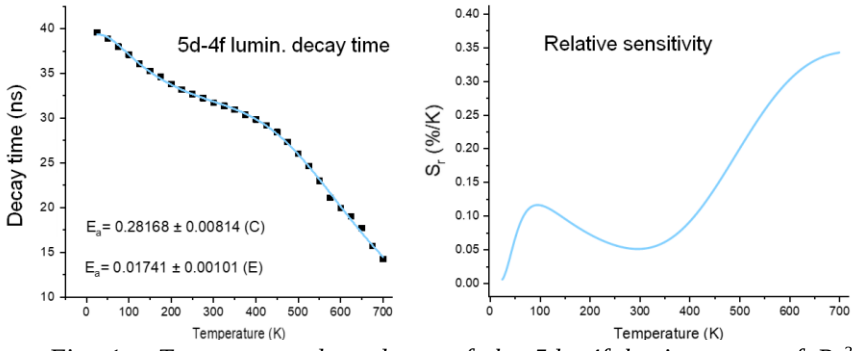

Fig. 1. Temperature dependence of the 5d→4f luminescence of Pr^{3+} in $Ca_3Sc_2Si_3O_{12}$:Pr and the relative sensitivity derived from the data.

Acknowledgments: This research was supported by the Polish National Science Center (NCN) under the grant #UMO2018/29/B/ST5/00420.

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