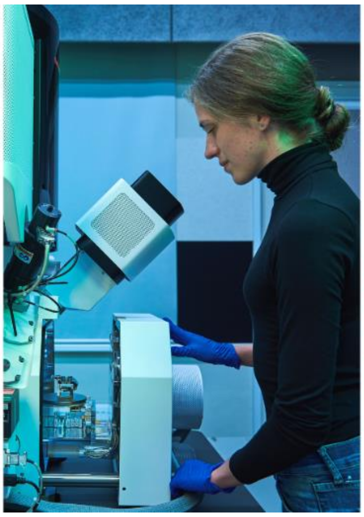
INSTITUTE OF SOLID STATE PHYSICS
UNIVERSITY OF LATVIA

RESEARCH PROGRAMME 2030






Riga

2025

FOREWORD

The global society faces environmental, social and economic challenges such as tackling climate change, efficient health systems, assessing the new alleys and inherent risks posed by the explosive development of artificial intelligence, the well-being and security problems, strengthening economic competitiveness, and creating jobs.

2024 was a year full of upheavals. The continuing war in Ukraine, the Middle East conflicts, China-Taiwan tensions, the outcome of the United States election, natural disasters remind us every day that our world is increasingly unstable and that predicting the future is becoming more and more difficult.

An increased focus on research in different defence-related technologies is expected in multiple technologies related to artificial intelligence and the rising dominance of drone warfare: sensors, secure communications, lasers, computer control, robotics, artificial intelligence etc. Research and development of dual-use technologies for both military and civilian security will be intensified.

This puts an additional focus on research fields, helping to reduce the dependence on fossil fuel energy and different raw materials (like rare earths, lithium etc.) imported from non-reliable or belligerent foreign suppliers. With a rapid development of solar and wind energy, energy storage diversity, like batteries and hydrogen-based technologies, become increasingly important.

New materials are the key to many global challenges. To tackle them, researchers must be able to develop advanced and sustainable materials with the required properties, to improve the recyclability of materials, reduce their carbon and environmental footprint and make sure that a wide community of users will be able to capitalize on them. The materials development cycle ending with components used in real applications is long and entails steps such as theory and modelling, the appropriate technology for obtaining them, characterization, up-scaling and engineering, including industrial environments, and driving cross-sectorial industrial innovation by supporting new applications in all industry sectors. To succeed, there is a need for research-innovation ecosystem with advanced research infrastructure and modern technological facilities.

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EXECUTIVE SUMMARY

Motto: ***Thinking together is a progress and working together is a success***

GENERAL INFORMATION ABOUT ISSP UL

The Institute of Solid-State Physics University of Latvia (ISSP UL) is an internationally recognized leader in material sciences and cross- disciplinary topics in Baltic Sea Region. Its scientific capacity and the research and innovation ecosystem are currently being further developed through EC Teaming project "The Centre of Advanced and Material Research and Technology Transfer" ($CAMART^2$) – (2017-2025). ISSP UL aims to transfer excellence in materials science and solid-state physics into innovative products, processes and services.

ISSP UL **Vision** is to be a world-class recognized Excellence Centre – an outstanding place for research and innovation.

ISSP UL **Mission** is to create a dynamic environment for solutions of global societal and technological challenges, strengthening the role of Latvian and European science in the world.

STRATEGIC RESEARCH AREAS

The main efforts in future advanced material studies at ISSP UL are specified in **three Strategic Research Areas:**

- Materials for photonic devices,
- Advanced materials for energy,
- Microfluidics and biomedical technologies

I. MATERIALS FOR PHOTONIC DEVICES

Polymer photonics integrated platform and quantum photonics.

Focus on:

- To create a set of standard modules that can be used to design and fabricate sensors, light sources/emitters, modulators, processors with high reproducibility.
- To develop integration of photonic platform with electronic and microfluidic devices to provide applications needed in most of the societal challenges: health, wellbeing, security, ICT, environment.
- To develop structures for edge and grating couplers.

Nonlinear optical (NLO) materials.

Focus on:

- Basic understanding of third - order and second-order NLO effects in organic materials.
- Development of Kerr effect evaluation through Quantum Chemical Calculations (QCC).
- Innovative approaches for development of materials for advanced All -Optica Devices.

Materials for low-loss optical fiber waveguides.

Focus on:

- The studies of factors limiting transparency of SiO_2 glass in ultraviolet, deep-ultraviolet and vacuum-ultraviolet spectral regions. This research is especially important in the context of developing wide spectral range and radiation/solarization-resistant optical fibers, which are required for analytical, medical, nuclear energy-fusion diagnostics and space applications.
- The studies of the effects of densification of silica on defect creation.

0D, 1D, 2D and mixed-dimensional nanomaterials.

Focus on:

- Photochromic, thermochromic, electrochromic advanced materials; technologies for fabrication of low_cost thin-film SW and chromogenic devices.
- Integrated over robot body discreate miniaturized proximity sensors together with tactile sensors.
- Development of 1D core-shell nanowire heterostructures with superconducting shell for quantum/optoelectronic applications.
- Nanomechanical experiment on smart actuation materials like pure VO2 and core-shell NWs.

Luminescent materials.

Focus on:

- The radio- and photoluminescence research of prospective scintillator materials as ZnO:In and ZnO:Ga..
- The research of materials for the luminescence dosimetry will be concentrate on Al_2O_3 based materials, AlN and wide gap dielectrics.

X-Ray Absorption Spectroscopy.

Focus on:

- The development of novel methodologies based on machine learning methods, enabling faster material simulations, decision-making, and real-time experiment control and their application to the study of smart and high-entropy materials.
- Combined with theoretical structure prediction tools based on ab initio quantum chemistry, such EXAFS experiments will accelerate exploring materials, such as thermochromic, electrochromic, photocatalytic and others for photonics applications, and discovery and enhance understanding of their properties.
- The study of materials under extreme conditions, such as ultra-high pressures and temperatures, what offers a path to discovering new materials not possible with conventional methods.
- The VUV excitation spectroscopy under synchrotron radiation is a powerful toll for the study of optical and luminescence properties of wide bandgap materials.

Surface-enhanced Raman Scattering (SERS).

Focus on:

- Replacing traditional FIB technology for production nanostructured SERS substrates by introducing sample under test into hollow core optical fiber.
- Application of SERS in other domains like microfluidic devicesfor targeted measurements of specific contaminants.

Ultra-wide bandgap semiconductors.

Focus on:

- The development of novel solar-blind far-UV light photodetector based on amorphous Aluminium Gallium Oxide (AlGaO).

Organic solid-state lasers and organic light- emitting diodes.

Focus on:

- Influence of metal nanoparticle surface plasmon resonance on amplified spontaneous emission (ASE) threshold values in organic materials.
- Investigation of organic NIR emitters with advanced characteristics, thus such properties could increase the applications of lasers in telecommunication, bioimaging and lab-on-chip.
- Developing the methods of depositing OLED on flexible substrate to broaden OLED applications.

Phase retrieval methods for adaptive optics, imaging and photonics.

Focus on:

- Development of computationally effective phase retrieval algorithms for optical applications, including holography, vision research and photonics.
- Implementation of novel type of wavefront sensors foreseen for biomedicine and astronomy.

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II. ADVANCED MATERIALS FOR ENERGY

Theoretical material science and modelling.

Focus on:

- Modelling materials for renewable energetics.
- Nanomaterials for water splitting and hydrogen production.
- Heterojunction photocatalysts for green hydrogen production by means of DFT supportedgenerative machine learning.
- Cathode materials and proton conductors for fuel cells transforming chemical energy into electricity. Modelling functional materials for the fusion reactors exposed to an intensive radiation and high temperatures.
- Dynamic self-sssembly of materials under harsh radiation conditions.

Materials for batteries.

Focus on:

- Electrodes for Li-ion /Na-ion batteries and supercapacitors.
- Active electrode materials; Inert protective coatings;
- Conductive additives and Ionic liquid-based electrolytes.
- Low temperature Ionic-liquid-based Li-ion battery cells.
- Commercial battery cells (performance vs. temperature, C-rate, etc.).

Hydrogen.

Focus on:

- Innovative catalyst and its regeneration for clean hydrogen production via methane pyrolysis.
- Aluminum recycling and related hydrogen production.
- Hydrogen sensing and quantification, Polymer membranes.

Organic and hybrid photovoltaics.

Focus on:

- Development of ternary organic solar cells.
- Development of hybrid chalcogenide/ organic tandem solar cells

Novel Thermoelectric Materials.

Focus on:

- Development of organic-inorganic hybrid system thin films for thermoelectricity;
- Development of Thermoelectric generators on a flexible substrate.

Thin film and coating technologies.

Focus on:

- Development of industrially scalable technologies for fabrication of low-cost thin film “smart windows (SW)” and chromogenic devices.
- electrochromic, photochromic, thermochromic, transparent conducting materials - roll-to-roll (R2R) magnetron sputtering system.
- Study the photochromic mechanism with the aim to optimize photochromic parameters, and to reduce degradation of material caused by humidity.
- Producing and study of RE-doped YHO films and multilayer coatings, including large-area coatings on polymer substrates produced using the R2R process.
- Testing of large area photochromic films in different geographical locations across Europe.

Ultra-wide bandgap semiconductors.

Focus on:

- Development the first spinel – rear earth-abundant and non-critical oxide materials – power electronics technology platform.
- Elaboration of UWBG ZnGa2O4, MgGa2O4 and MgAl2O4 spinel epilayers with electronic properties required for their application in beyond the state-of-the-art high-power (> 6-10 kV) rectifiers and metal oxide semiconductor field-effect transistors (MOSFET) devices.
- Development of vacuum thin film deposition technologies for the stable deposition of gallium oxide (Ga_2O_3) and $ZnGa_2O_4$ thin films by reactive pulsed-DC magnetron sputtering from a liquid Ga target.

Novel lead-free and low-dimensional ferroelectric materials.

Focus on:

- Development of novel functional ferroelectrics and low-dimensional structures for flexible sensors, and energy harvesting.
- Study of zero-, one-, and two-dimensional ferroelectrics, such as $CuInP_2S_6$ thin films and nanoflakes, aiming to optimize polarization switching and piezoelectric properties.
- Analysis of influence of core-shell structure on physical properties (impedance, domain structure, resistance to electrical breakdown, and fatigue.
- Advancements in both high-tech and biomedical sectors while promoting innovation in eco-friendly, lead-free ferroelectrics.

III. MICROFLUIDICS AND BIOMEDICAL TECHNOLOGIES.

Prototyping of microfluidic devices.

Focus on:

- State Research Programme "Innovation Fund Long-Term Research Programme" Project "Biomedical and Photonics Research Platform for Creating Innovative Products" **(BioPhotT).**

- Development an Organ-on-Chip (OoC) – a microfluidic device that can model the biology of human organs to advance biomedical research and drug development.
- Development of multiple models supporting necessary design changes, including sensor integration (TEER, O_2, CO_2, pH) and membrane engineering to support 3D cell arrangements.
- Dedvelopment of TEER sensors correlating TEER values with tight junction protein expression in gut-on-chip models and a novel biomaterial test bed recapitulating a rodent calvarial critical-size defect model in an OoC platform.

Materials for biomedical applications.

Focus on:

- Biomarker research of extracelluar vesicle (EV) technology for cancer diagnostics and treatment.
- Development of new low temperature synthesis methods for doped carbonate/phosphate materials for biomedical applications and comprehensive characterization of the obtained materials, based on persistent luminescence observed under different types of excitations (UV – visible light, X-rays etc.).
- Evolve studies of transprent conducting coatings with antimicrobial properties: WO3/Cu/WO3, ZnO/Cu/ZnO.

RESEARCH PROGRAMME

We are making progress

Research Programme is a dynamic, regularly updated document which serves as a supporting roadmap for the Intstitutes **Research Strategy**.

The current **Research Programme 2030** includes updates of a few **Research domains** to explore new innovative and interdisciplinary fields of science, defined at **national level** as **RIS3** areas:

- "Photonics, smart materials, innovative products and technologies"'.
- "Biomedicine and biotechnology".

At **international level,** the **Research Programme,** and the corresponding **Domains** within it, addresses the scientific, research and innovation challenges aligning with **Horizon Europe** and **EURATOM Programme,** and in sustainable outlook with **FP10 Programme 2028-2034**.

The outline of each **Research Domain** is organized according to the progress in each of the subsections **-** "State of the art", "Our position", "Future activities", "Networking", and "References".

The following sections provide description of the 24 research domains.

MATERIALS FOR PHOTONICS AND ELECTRONICS

POLYMER PHOTONICS INTEGRATED PLATFORM AND QUANTUM PHOTONICS

State of the art

Integrated circuits are essential parts of almost all modern technologies from personal computers, medical devices to cars and spacecrafts. Much of the functionality of these electrical components can be replaced with photonic components to create photonic integrated circuits, which use light instead of electrons. Higher speed, lower energy consumption and greater bandwidth are just a few advantages as compared to conventional circuits.

In the last couple of decades, huge effort has been put into the development of photonics platforms based on various materials such as Si, Si_3N_4, InP, $LiNbO_3$, GaAs and others. Only few of them (Si, Si_3N_4, InP) have turned into eco-systems resembling semiconductors industry of design house, foundries, fabless companies and multi project wafer (MPW) services of photonics integrated circuits (PICs). Silicon photonics is the dominant mostly due to compatibility with CMOS process and MPW services are offered by multiple parties: IMEC, CEA-LETI, IHP, AIM Photonics and others. Silicon nitride photonics is gaining ground owing to the broad wavelength range starting from visible wavelengths allowing applications also in biophotonics among tele/Datacom and optical signal processing. MPW services of silicon nitride photonics are provided by IMEC, CEA-LETI, LionX, IMB-CNM and others [1]. InP allows possibility to implement both active and passive devices on a single chip. MPW services of InP PICs are provided by Smart Photonics and Fraunhofer HHI [2]. While various photonic platforms have matured to industrial level, they still have numerous challenges including limits set by material properties, expensive fabrication and complicated hybrid integration.

Polymer materials provide numerous advantages over semiconductor and oxide/nitride platforms:

1) Combination of passive and active elements [3];

2) Integration of other elements for hybrid and heterogeneous platform;

3) Losses;

4) Wide wavelength range [6];

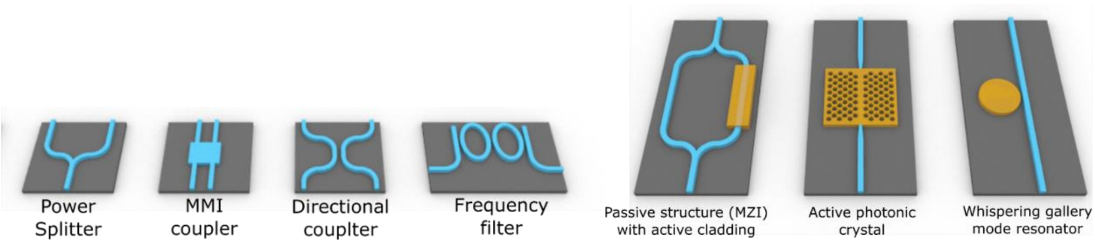
5) Multilayer structure [7];

6) Applications [8-10].

Polymer Photonics Technology Platform offers standardized polymer photonic device preparation methods to academia and industry. This system is based on three main parts: computational simulations of optical devices, materials and element fabrication workflow, and producible photonic elements.

Fabrication methods are separated into three groups: passive element fabrication, active element fabrication, and optical coupling elements. Since all waveguides are in size over one micron, conventional photolithography will be used to define structures. Both direct development and dry etching is used to produce passive elements. Straight sidewalls are offered to minimize losses.

Photonic elements (waveguides, power splitters, directional couplers, frequency filters, MMI couplers, passive cladding, active cladding, resonators, photonic crystals, grating couplers, edge couplers) are based on selected materials and fabrication workflows a library of basic photonic elements has been compiled including specific design rules for each element.



Passive elements and active elements

Single-photon and correlated photon pair sources are critical components in quantum technologies, such as quantum cryptography, quantum computing, and quantum communication. These sources enable secure data transmission and computational processes that rely on the properties of individual photons, such as superposition and entanglement. The search for efficient, tunable, and scalable single-photon sources has brought organic materials to the forefront, thanks to their unique optical properties, ease of synthesis, and tunability.

Organic molecules have shown significant promise in single-photon and correlated photon pair generation due to their high quantum efficiency, tunable emission wavelengths, and ease of integration into diverse platforms. Organic molecules such as fluorescent dyes like, DBT, TBT, TDI etc. [14] are particularly promising for single-photon emission due to their well-defined excited states and ability to emit photons upon excitation. When a single organic molecule is excited by a laser, it can undergo radiative decay, resulting in the emission of a single photon. This property makes organic molecules ideal candidates for single-photon sources that can operate at room temperature, a significant advantage over other systems such as quantum dots and color centers in diamond, which often require cryogenic conditions for efficient operation.

Correlated photon pair sources are essential for generating entangled photon pairs, a key resource in quantum cryptography and quantum teleportation. Entangled photons exhibit non-classical correlations, meaning that the measurement of one photon's state directly influences the state of its entangled partner, no matter how far apart the two photons are. Organic materials have shown potential in generating correlated photon pairs through processes such as spontaneous parametric down-conversion (SPDC) and four-wave mixing (FWM). Polymers like poly(methyl methacrylate) (PMMA) and polycarbonate have been used in waveguides and microcavities to enhance the efficiency of SPDC. These polymers are often doped with nonlinear organic dyes to increase their optical nonlinearity. Additionally, organic crystals like DAST (4-N,N-dimethylamino-4'-N'-methyl-stilbazolium tosylate) [15] have been utilized for their strong nonlinear coefficients, allowing for efficient photon pair generation in compact devices. The use of organic materials in SPDC-based photon pair sources has the potential to make entangled photon sources more scalable and integrable into quantum communication systems.

Our position

Laboratory of Organic Materials has vast experience regarding third-order nonlinear optical organic material studies [16,17], optical gain materials as well as the expertise in polymer thin-film fabrication. In last year's research has also shifted towards photonic device designing and fabrication leading to demonstration of organic electro-optical switches [18] and all-optical gas sensor [19].

Standard workflows for optical lithography and mask aligner have been established allowing to create SU-8 structures down to 1 um. Further look in collaborations with chemists and biologists regarding polymer sensor development for specific applications will be performed.

COMSOL software packets are available and a team responsible for simulations is being established. First works regarding simulations of polymer waveguide sensors based on lossy-mode resonance have been published.

We are also working on photonic device fabrication using dry etching, EBL, and trench structures.

In parallel to element fabrication composite photoresists were developed which consisted of photoresist and nanoparticles to improve photonic element fabrication with organic materials. [20]

Recently Laboratory of Organic materials has started quantum photonic s scientific direction. Previously investigation nonlinear optical organic compounds and organic laser compounds could be used in quantum photonics. Moreover, quantum photonics could be combined with the Polymer Photonic Platform. One of the strong positions is collaboration with chemist groups that allow to design and synthesise new materials for single photon and entangled photon sources.

Future activities

The aim of the photonics platform is to offer a modular set of elements, repeatable technologies and materials needed to create photonic elements for wide range of applications. Ultimate goal is to create a set of standard modules that can be used to design and fabricate sensors, light sources/emitters, modulators, processors with high reproducibility, predictable budget and time. Photonic platform should be integrated with electronics and microfluidics to provide applications needed in most of the societal challenges: health, wellbeing, bioeconomy, security, ICT, environment.

Special attention will be given to structures for edge and grating couplers. In case of edge coupling, light is coupled in and out from the waveguide from its facet using a fibre. This technique usually requires optical quality facets for high coupling efficiencies. This technique not only allows high efficiency, but also broad bandwidth and polarization independence. Disadvantages include larger footprint than grating couplers, fixed coupling positions, and requirement for edge polishing [21]. To increase coupling efficiency facet couplers our team can offer facet polishing, specific taper designing, on-chip groove etching for fibre alignment and optimal coupling angle calculations. We have developed a procedure for waveguide polishing and fiber attachment to waveguide facets, but this procedure needs further optimization to yield lower coupling losses.

Networking

Latvia:

- Riga Technical University, prof. Valdis Kokars, assoc. prof. Kaspars Traskovskis, prof. Sandis Spolitis;
- University of Latvia, assoc. prof. Jānis Alnis.

Abroad:

- Italy: University of Trento, prof. Lorenzo Pavezi;
- France: University of Technology of Troyes, prof. Christophe Couteau.

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NON-LINEAR OPTICAL EFFECTS, MATERIALS AND DEVICES

State of the art

In the last years third-order nonlinear optical materials have seen a new rise in interest due to the development of soliton microresonators [1] for microwave applications, telecommunications, and optical sensors as well as for quantum photonics [2] with the main focus on entangled photon sources and non-destructive photon interaction. In all of these technologies materials with a strong Kerr effect play a key role [3]. One of the main limitations for this technology transition from laboratory tests to commercial applications is the lack of efficient materials with strong Kerr effect and low optical losses. On the other hand, materials with high optical loses due to strong Two-photon absorption (TPA) can be used in optical limiting applications. In case of developing slow thermo-optical switches materials with a strong thermo-optical effect is desirable. At same time for ultra-fast all-optical switches pure electronic part of the Kerr effect is essential and the interference from other effects must be limited. Although there are plenty of published papers about Kerr effect estimation [4–5], distinguishing between thermo-optical and Kerr effects, separating Kerr effect into fast electronic response and slower molecular effects and evaluation of relaxation time for each effect are among important methodological problems in investigations of third-order nonlinear optical materials [6].

For practical application mainly two third-order NLO effects have been considered – Kerr effect and Two-photon absorption. The main issue with third-order NLO studies is the correct interpretation of nonlinear refractive index changes – are they induced by thermo-optical or Kerr effect and how large are each of the Kerr effect components – electronic, vibrational and reorientational. To study these effects, the term Optical Kerr spectroscopy has been present in the scientific literature for a while [3]. Most of these works are mainly based on Beam-Deflection or specific Pump-probe measurement methods to study temporal and some spectral aspects of Kerr effect. At the same time, many publications have already indicated that pulse repetition rate [5], polarization resolved Z-scan [7] and other measurement methods can give significant information about nonlinear refractive index of material absent from the previously mentioned Optical Kerr spectroscopy works. Recently much attention has been given to application of Laguerre–Gaussian vortex beams in NLO studies [8]. While most of literature has been focused on third-harmonic generation studies scientists are slowly exploring possibility to use vortex beams in Kerr studies [9].

For practical all-optical device implementation, it is necessary to achieve a high confinement of light. To realize such confinement, typically waveguide and photonic crystal devices are considered. Despite that the subject of all-optical devices is growing in popularity, only some experimentally validated examples have been demonstrated as summarized in the review article [10]. Current state-of-the-art includes few examples of devices using graphene for optical switching [11] or polariton opto-optical devices using organic materials [12]; even so, these devices are still in early development phase. Due to the low efficiency of available third-order materials, just a limited amount of waveguide devices have been experimentally validated and reported. The most common include whispering gallery mode (WGM) resonators and photonic crystal cavities [13-14] which have been used in sensing, communications, spectrometry and other applications.

Our position

The competence of Laboratory of Organic Materials allows dealing with the main issues related to studying properties and assessing applications of NLO materials. We have broad experience in structure-property relation studies of second- [15–17] and third-order[18,19] NLO organic materials. Along with these studies, we have gained experience in performing Quantum Chemical Calculations (QCC) to obtain first and second-order hyperpolarizabilities of organic materials.

Great attention has been given to development of experimental methodology for investigation second-order [20,21] and third-order NLO [18,22,23] properties. Development of polarization-resolved Z-scan measurements [24] allows us to study in more detail the origin of Kerr effect in specific media. This is especially essential as only the electronic part of Kerr effect is applicable for high-bandwidth all optical processing.

Laboratory of Organic materials has conducted research to create photonic devices based on SU-8, PMMA and active NLO organic materials. By combining SU-8 as passive material for optical waveguides with guest-host system of active NLO chromophores and PMMA as active materials, we have been able to demonstrate functioning electro-optical switch [25] as well as all-optical gas sensor [26]. Recently we have begun to study NLO properties of nanoparticles and quantum dots. This includes both silver nanoparticles [23] as well as more complex materials such as HgTe [27], HgS [28], Bi_2Te_3 [29] and $ReSe_2$ [30]. These researches have also extended to studies about silver nanoparticle influence on reorientation Kerr effect of organic chromophores have been published [24]. Recently we have also started to study near-zero-epsilon materials with main focus on ITO nanoparticles and their usage for NLO applications [31].

Future activities

The important goal of future activities will be acquiring new knowledge that will contribute: a) to basic understanding of third-order NLO effects in organic materials; b) to develop correct measurement methodology to characterize their NLO properties. This could lead to new structure–property studies and third-order NLO organic materials designs. Moreover, the planned development and verification of Quantum Chemical Calculations (QCC) methods for third-order NLO material property calculations could lead to faster molecule screening. To work on better fundamental understanding of nonlinear optical effects we have started work on fifth-order Kerr effect studies focusing on solvents and novel organic dyes that exhibits this response in 600-800 nm spectral window. Parallel to that we study strong Kerr response in mediums that has their absorption saturated for low-loss nonlinear optical mediums.

Development of measurement methodology

Measurement methodology developments include:

- Polarization-resolved Z-scan measurements;
- Beam-deflection method;
- Fluorescence anisotropy measurements.

We have established both Polarization-resolved Z-scan method for spectral measurements and Beam-deflection method. First experimental results regarding spectral Z-scan measurements have been published [21,22]. Next planned measurement methods are:

- Third-harmonic generation.
- Vortex beam application in measurements.

Development of Kerr effect evaluation through Quantum Chemical Calculations (QCC)

Use of reliable QCC for predicting and/or describing non-linear optical properties of materials allows to improve significantly the efficiency of the structure screening through rationalizing the structure–property relationships. By means of QCC we plan to obtain:

- ***Linear polarizability values,*** which allows us to estimate reorientation contribution;
- ***Raman scattering intensities and frequency,*** to calculate the vibration contribution;
- ***Second-order hyperpolarizability*** values, which allows us to calculate the electronic contribution.

For reorientation and vibration effects additional attention will be given to time constant calculations [7].

Second-order NLO materials

Parallel to study of third-order materials, we also do part of research in second-order material studies that includes ferroelectric materials [32] as well as study of novel organic dyes for electro-optical applications.

Networking

Latvia:

- Riga Technical University – Institute of Applied Chemistry;
- Ceram Optec optical fiber company;
- Laboratory of Nonlinear Optics, UL, Rashid Ganeev;
- Quantum Optics Laboratory, Janis Alnis;
- Latvian Institute of Organic Synthesis, Kaspars Leduskrasts;

Abroad:

- Lithuania: Kaunas University of Technology - Faculty of Chemical Technology;
- Switzerland: Swiss Federal Institute of Technology Lausanne – Photonic Systems Laboratory;
- Taiwan: National Sun Yat-sen University;

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OPTICALY ACTIVE DEFECTS IN SILICON DIOXIDE

State of the art.

A wide range of optical and photonics applications demand low-loss optical fiber waveguides, deep-ultraviolet (UV) transmitting optics, optical components capable of operating in ionizing or particle radiation environments, and elements that can transmit high-power laser light. In most cases, the optimal material for these purposes is pure or doped glassy SiO_2 (silica glass). With a wide band gap of approximately 9 eV—the largest among all glassy materials—silica is the preferred choice for three important groups of applications:

- Optical components and devices operating in the ultraviolet (UV) spectral range, such as windows, lenses, filter and grating substrates, thin-film coatings, and UV fiber waveguides [1];
- High-power optical applications, ranging from fibers used in laser surgery or metal welding [2] to femtosecond laser writing [3], and to lenses for laser-ignited nuclear fusion [2];
- Photonics devices made from glassy SiO_2, which are highly resistant to radiation damage and are extensively studied for use in nuclear energy and space applications [3,4]. The development of hollow-core fibers [5] holds promise for even higher power transmission and greater resistance to radiation. In 2021, an ultra-stable, high-density "5D" data storage—achieving multi-terabyte capacity—was demonstrated through femtosecond laser writing in silica glass [11].

A critical phenomenon underpinning all these applications is the presence or formation of optically active point defects in the material. This issue has been extensively studied, and a significant level of understanding has been reached (see, for example, reviews [3,4,6]). However, several challenges remain unresolved. These include identifying the exact origins of defect-related absorption in the deep UV region, understanding the influence of technological impurities such as chlorine and carbon, examining the incorporation of fluorine and related defects in highly fluorine-doped SiO_2 glasses, and assessing the impact of internal surfaces in the amorphous structure of SiO_2 on its optical and photochemical properties.

Recently, several research and review papers [14-17] highlighted a new trend focused on densifying silica-based glasses and engineering the size of nanovoids inherent to their structure. This has become a prominent area of research aimed at further enhancing the transparency of optical fibers used in long-range communication. At the currently achieved level of glass purity, Rayleigh scattering caused by density fluctuations in the glass is the primary source of signal attenuation in optical fibers. It has been found that these density fluctuations can be minimized by hot-pressing silica glasses [14], a method now being explored by multiple research groups. In addition to this emerging trend, there is continued strong interest in femtosecond laser writing in silica glass, particularly for Bragg gratings and data storage applications [17-21].

Our position

Researchers of the Laboratory of Optical Materials have detailed knowledge and long experience with SiO_2-based optical materials. Their past work has been crucial for identification and establishing of optical properties and radiochemical transformations of a number of basic defects in glassy SiO_2, like oxygen dangling bond ("non-bridging oxygen hole center", NBOHC), divalent Si ("silicon oxygen deficiency center", SiODC), interstitial hydrogen H_2, oxygen O_2 and O_3 (ozone) molecules in SiO_2. They have authored several well-cited reviews on this field (see, e.g., ref. [6] and references therein).

More recently, this group has tackled the problems of chlorine, a widespread and detrimental technological impurity in synthetic SiO_2 made from $SiCl_4$ [7,12], the dynamic properties of O_2 molecular interstitials in SiO_2 [8] and the similarities and differences of defects in crystalline and glassy SiO_2 [9]. The group has identified a number of up-to now not understood carbon-related defects in silica, demonstrating that they are due to interstitial polycyclic hydrocarbons [13]. A PhD student now works on closely related topics. Most recently, in 2023, this group identified the first paramagnetic defect in fluorine-doped silica, directly linked to fluorine [25].

The group possesses strong expertise in optical, vibrational, and magnetic spectroscopies. They utilize both custom-built equipment, such as vacuum-UV spectrometry, thermally stimulated luminescence, and radioluminescence, as well as the recently upgraded general-use equipment at ISSP UL. Additionally, the group has recently added in-laboratory sol-gel synthesis of silica glasses to its capabilities.

Future activities

- Studies of factors limiting transparency of SiO_2 glass in ultraviolet, deep-ultraviolet and vacuum-ultraviolet spectral regions. This problem is most important in the context of developing wide spectral range and radiation/solarization-resistant optical fibers, which are required for analytical, medical, nuclear energy-fusion diagnostics and space applications.

- Studies of chlorine- and carbon- related defects in SiO_2 – based glasses. Presently, a transformation from chlorine-related to carbon-related technology in the synthesis of SiO_2 glasses is gradually taking place. This is caused in part by ecological considerations and in part by the detrimental effect of Cl trace impurities on optical properties and solarization resistance of SiO_2 glass and optical fibers. While the properties of Cl impurities are known to some extent [7,12], the nature and optical properties of carbon dopants are much less understood.

- Based the results of the recent work [13], particular activity will be focused on polycyclic hydrocarbons as optically active dopants in silica glass and on their possible role as precursors to other carbon-related defects and carbon nanodots.

- Studies of fluorine-related defects in glass. Fluorine is widely used in optical fiber technology to decrease the refraction coefficient and/or to reduce the fictive temperature of glassy SiO_2. Fluorine doping is presently studied as a way to further reduce the Rayleigh scattering in ultra-low loss optical fiber waveguides [10]. It generally increases the radiation resistance of the glass [2]; however, this effect decreases at large F concentrations. Relying on the recently discovered electron paramagnetic resonance (EPR) evidence for fluorine-related defects [25], their optical properties and the nature of their precursors will be studied. This knowledge is needed in order to optimize the optical fiber technology.

- Studies of the effects of SiO_2 glass morphology on the optical and photochemical properties of the material. Amorphous SiO_2 can be obtained in a large number of different forms with different morphologies (nanoparticles, nanofibers, nanoporous, micro- and mesoporous materials, porous crystalline (zeolite-like) structures. These materials possess large internal surfaces facilitating their use in chemical and biomedical applications.

- Developing of experimental capabilities supportive to the R&D needs of Latvian fiber optics industry. Performing of contract works on optical fiber spectroscopy. Joint ERDF projects.

- In view of the perspective of using nanoscale defect structures in silica for long-term information storage [11], it is planned to focus on studies of the properties of defects in silica induced within internal nanovoids, created by laser damage or high energy nuclear irradiation.

- Defects created by ion implantation of silica (in collaboration with KTH, Sweden).

- The studies of the effects of densification of silica on defect creation, in collaboration with Ecole Politechnique, France [20] will be continued.

Networking

- Collaboration with industrial partner in Latvia, Ceram Optec. A joint paper has been published in 2023 and an ERDF collaboration project has been submitted for 2025.

Internationally, the group has long-standing active collaborations with research groups in:

- France: Prof. Sylvain Girard, Youcef Ouerdane (Univ. Saint-Etienne), Dr. Nadege Ollier (Ecole Polytechnique, University of Paris-Saclay);
- Japan: Prof. Koichi Kajihara (Tokyo Metropolitan University), prof. Hideo Hosono (Tokyo Institute of Technology);
- Italy: Prof. Marco Cannas, Simonpietro Agnello (Palermo University);
- United Kingdom: Prof. Peter Kazansky (Southampton University);
- Sweden: Prof. Andres Hallén (KTH) .

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0D, 1D, 2D AND MIXED-DIMENSIONAL NANOMATERIALS

State of the art

Nanomaterials are defined as materials with at least one spatial dimension in the scale of 10^{-9} m, or usually below 100 nm [1]. They exhibit physical and chemical properties different from their bulk counterparts due to the large surface/volume ratio and, thus, the important contribution of surface atoms, as well as quantum confinement and other quantum phenomena [1]. Nanomaterials are classified by the number of dimensions in the nanoscale. 2D materials have one dimension below 100 nm, 1D and 0D materials have 2 and 3 dimensions in nanoscale, respectively. Examples are nanoparticles and quantum dots (0D), nanowires and nanotubes (1D), layered van der Waals materials (2D).

Zero-dimensional (0D) nanomaterials are the cornerstone of nanotechnology. Due to the inherent structural properties of 0D nanomaterials, such as ultra-small sizes and high surface-to-volume ratios, they have more surface area per unit mass. The high surface-to-volume ratio and quantum confinement effects of 0D nanomaterials provide improved or novel properties such as, for example, high photoluminescence (PL) quantum efficiency and enhanced catalytic activity. Various 0D nanomaterials have been extensively explored: carbon-based quantum inorganic quantum dots (QDs), magnetic nanoparticles, noble metal nanoparticles, upconversion nanoparticles. 0D nanomaterials have numerous potential applications in materials science, photovoltaic science, catalysis, energy, sensing, biomedicine and ink-jet printed devices [2].

1D nanostructures - nanowires (NWs) and nanotubes (NTs) – are being explored as promising materials for applications in electronics, optoelectronics, photonics and microelectromechanical systems (MEMS) [3]. Two different approaches of NW integration in devices are used – single-NW devices consist of individual separate NWs, whereas “bulk” devices contain periodic NW arrays or randomly dispersed NWs. The challenge is to develop a scalable device fabrication process that could compete with current technologies, such as silicon microfabrication. This is an active research field. Several concepts have been proposed, for instance, controlled printing of NWs with roll-to-roll technology that uses microfluidics to align the NWs [4]. Besides upscaling problems, the current 1D materials research focuses on finding new NW-based materials and studying their fundamental properties for novel applications [5]. NW characteristics can be engineered by creating core-shell heterostructures – modifying NW by a thin (compared to the diameter of the NW) coating of a different material [6]. Surface of NWs has a significantly reduced lattice mismatch restriction compared to conventional semiconductor thin film growth thus enabling greater flexibility in choosing the materials to produce heterostructures and in engineering their properties [7,8].

2D layered van der Waals (vdW) materials have attracted great interest since the isolation of monolayer graphene in 2004, due to their unique structure and the promising physical properties that appear when the thickness of the material is reduced to one atomic layer. These materials have an atomic structure similar to well-known graphite – strong in-plane bonds and weak interlayer bonding [9]. Bulk materials of this group have been widely studied in the last century, as most of these materials are quite abundant and have been used in different technological fields, however until 2004 it was believed that it is not possible to obtain an only one separate stable layer [10]. There was some research done in 1960s that showed that electrical conductivity in a few-layer graphite is higher when measured laterally in-plane rather than between the planes, but it was still assumed and assumptions justified by experimental and theoretical research that stable two-dimensional (2D) atomic crystals cannot exist separately in nature, as all attempts to obtain such were unsuccessful – with the used methods the layers tended to curl, roll or deform in other ways [11–13]. The ground-breaking discovery by K. Novoselov and A. Geim in 2004 proved otherwise – by mechanically exfoliating highly crystalline graphite with a Scotch tape they were able to obtain one atomic layer of graphite (graphene) on an oxidized silicon substrate and measure its electrical properties [10]. Graphene exhibits extraordinary electrical and mechanical properties [14]. For their contribution, Geim and Novoselov were awarded The Nobel Prize in Physics in 2010. Afterwards, 2D materials became one of the “hottest” topics in modern physics – in 2011 an intensive research started on layered transition metal dichalcogenide (TMD) semiconductors, mainly MoS_2 and WS_2 [15–17], and around 2015 more exotic compounds were started to be studied, such as NbS_2 and ReS_2 [18,19].

TMDs are described by a general chemical formula MX_2, where M is a periodic table Group 4 – 7 transition metal and X is a chalcogen, and have a potentially useful property of thickness-dependent bandgap [20]. TMDs layers have terminated surfaces without dangling bonds, bound together by weak vdW forces, therefore, they can be sequentially stacked unstrained without any covalent interlayer bonding and even if materials are slightly lattice-mismatched [21]. Large-scale synthesis methods of TMDs on different substrates need to be developed, before any practical applications could be realized.

The family of 2D materials includes several subgroups, classified by materials chemical formula and atomic structure: (1) transition metal dichalcogenides (i.e. MoS_2, WSe_2) and their related compounds (2) group IIIA chalcogenides (i.e. GaS, InSe) and (3) Group IVA dichalcogenides (i.e. SnS_2), most of these compounds are semiconductors, semi-metals or metals; (4) insulator hexagonal boron nitride (h-BN); (5) black phosphorus; (6) X-enes (i.e. graphene, germanene); (7) MX-enes (transition metal carbides and nitrides); and other compounds, such as few oxides, halides etc. [22–24] Some of these materials are naturally occurring, however some are only synthesized chemically, h-BN for example.

Combining NWs and TMDs in core-shell heterostructures could lead to new knowledge about the interface formation between different materials and solid-state reactions in such systems, to novel nanostructures with enhanced properties, and development of new TMDs synthesis methods as NWs are a convenient template to study materials growth.

Our position

One of our research topics is synthesis and investigation of mechanical and tribological properties of 0D and 1D nanomaterials (nanoparticles, nanodumbbells, nanowires, nanotubes) using Scanning Probe Microscopy and in situ nanomanipulations inside SEM [25-30].

As an example of unusual behaviour of nanomaterials, can be mentioned stress induced reversible plastic deformation or kink formation in CuO nanowires, published this year [26]. This work reports for the first time the post-synthesis formation of such defects, achieved by exploiting a peculiar plasticity that may occur in nanosized covalent materials. Specifically, in this work the authors found that single-crystal CuO NWs can form double kinks when subjected to external mechanical loading. Both the microscopy and atomistic modelling suggest that deformation-induced twinning along the (110) plane is the mechanism behind this effect. In a single case the authors were able to unkink a NW back to its initial straight profile, indicating the possibility of reversible plasticity in CuO NWs, which is supported by the atomistic simulations. The phenomenon reported here provides novel insights into the mechanisms of plastic deformation in covalent NWs and offers potential avenues for developing techniques to customize the shape of NWs post-synthesis and introduce new functionalities.

Another research topic is 2D materials and 1D-2D mixed-dimensional materials or core-shell NWs, there the shell is made of layered 2D materials (WS_2, MoS_2, ReS_2, PbI_2, $TaSe_2$, etc.). We found that the combination of properly chosen materials can bring improved and advanced properties of these NWs [31]. TMDs like WX_2, MoX_2, ReX_2 (X=S or Se) can be synthesized from metal oxide precursors (WO_3, MoO_3, ReO_3), however some transition metal oxides have too high chemical stability to use them as precursor (e.g., Ta_2O_5 and TiO_2). We developed a method of TMDs synthesis from metal precursors [32-35]. However, properties of metal oxide and metal precursor derived TMDs films may differ significantly. For example, $ReSe_2$ thin films can be produced from magnetron sputtering of Re and ReO_x on flat substrates with subsequent selenization via atmospheric pressure chemical vapor transport (CVT) [32]. Some metals like Ta, Ti, V can be converted into TMDs in vacuum sealed ampoules only (conversion at atmospheric pressure is not efficient). $TiSe_2$ and VSe_2 thin films can be prepared in vacuum sealed ampoules from Ti and V metal film precursors in temperature range 650-750 °C [33]. They temperature-dependent local structure and lattice dynamics was also probed by X-ray absorption spectroscopy [34]. Last but not least study was performed on metallic Ta shell selenization of core-shell ZnS/Al_2O_3 nanowires [35]. Thin alumina shell coated by ALD help to encapsulate and stabilize ZnS nanowires from unwanted morphological changes during selenization of Ta coating at 650 ºC inside a vacuum-sealed quartz ampoule and to produce high quality ZnS/Al_2O_3 $TaSe_2$ core-shell NWs.

Future activities

There are three main activities of ISSP UL in field of nanomaterials are planned in near future:

- **Synthesis and application of 0D nanomaterials for ink-jet functional printing,** Functional ink-jet printing is a promising new technology, cheap and environmentally friendly, and creates a new paradigm in digital manufacturing where electronic devices and circuits can be printed on demand. Our main goal is a development and demonstration of the ink-jet technology, able to print flexible functional electronic devices. A complex "kit" of functional inks based on 0D nanomaterials (electroconductive, luminescent, thermochromic, semiconducting nanoparticles and others) will be developed to implement this technology. Printing of electronic components and simple electronic devices (connecting wiring, resistors, capacitors, transistors) will be used to develop printing and post-processing protocols for each ink type. Another important application of functional inkjet printing is chromogenic coatings for smart windows.

- **Development of 1D core-shell nanowire heterostructures with superconducting shell for quantum/optoelectronic applications**. We are developing technology of superconducting coatings based on MgB_2 material and hybrid superconducting nanowire synthesis with goal to create nanomaterial suitable for photodetection in broad wavelength range. It is planned to experimentally investigate the effect of strain in MgB_2 nanocoatings on its superconductivity transition temperature using various approaches of strain engineering in a core-shell nanowire (NW) configuration, including epitaxial mismatch strain, interstitial impurity strain and nanomechanical tensile tests of individual NWs in situ cryostat.
- **Nanomechanical experiment on smart actuation materials like pure VO_2 and core-shell NWs.** Smart actuation materials (SAM) able to convert external stimuli, including heat, light, electric current to mechanical motion. Metal-to-insulator or MIT materials can be scaled down to nano-dimensions without any loss of actuation properties. Investigation of 1D nanostructures MIT materials properties, and their integration into NEMS devices are of great scientific interest and will enable further actuator device miniaturization and higher operation speed. We are planning to produce and explore actuation properties of advanced MIT materials based on pure and doped VO_2 thin films and nanowires for MEMS and NEMS technologies for increased operation speed and application-defined working temperature.

Networking

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ELECTROLUMINESCENCE AND ORGANIC LIGHT-EMITTING DIODES

State of the art

A significant portion of overall energy consumption is attributed to lighting and displays. Achieving highly efficient artificial lighting with favourable spectral characteristics remains a major challenge. Organic Light-Emitting Diodes (OLEDs) present a viable solution in these areas. Such diode systems can be integrated into Smart Cities and energy-efficient buildings. Artificial lighting could be incorporated into windows or ceilings, while smart TVs and displays could be embedded in mirrors or walls. These implementations have the potential to drastically reduce energy consumption several times over [1,2,3]. The number of publications featuring the keyword "OLED" has surged from just 6 in 1996 to 2,293 in 2023 (according to the SCOPUS database). Concurrently, OLED technology has gained a significant market share in areas like OLED displays and lighting. The projected market revenue for OLED displays is expected to reach 82 billion USD this year, with further exponential growth anticipated over the next decade (data from the 360 Research Report). However, many unresolved challenges are slowing down the accelerated growth of this technology.

Over the years, the development of suitable light-emitting organic molecules has been the primary driver behind OLED technological progress. Initially, OLEDs used fluorescent compounds, but it quickly became evident that these first-generation (G1) emitters had fundamental limitations. Due to the spin state recombination process, electric charge excitation of organic molecules produces excited states, 25% of which are singlets (S), while 75% are triplets (T) [4]. In G1 emitters, only singlet states are emissive, as the spin-forbidden T1→S0 transition prevents triplet states from radiatively decaying.

It wasn't until 1998 that researchers demonstrated the potential to achieve 100% internal quantum efficiency using second-generation (G2) phosphorescent emitters [5]. Structurally, G2 materials are organo-metallic compounds featuring a heavy transition metal atom. The presence of this metal atom induces a process called spin-orbit coupling (SOC), drastically altering the photophysical behavior of the molecules. Due to the fast intersystem crossing (ISC), all excited states in these compounds rapidly transition to the lowest-energy triplet state (T1) [4]. Instead of being non-emissive, radiative relaxation occurs as phosphorescence because SOC enables mixing of singlet and triplet states, making the T1→S0 transition possible. Phosphorescence lifetimes (τ) in G2 compounds typically range from 1.5 to 5 microseconds, compared to seconds-long lifetimes for purely organic fluorophores. This allows OLEDs based on G2 emitters to utilize all excited states, boosting the device's internal quantum efficiency from 25% to 100%. Transition metals like osmium, rhenium, rhodium, platinum, and iridium are commonly used to synthesize these materials, with iridium and platinum being the most widely applied. To date, G2 emitters remain the industry standard due to their relatively short emission lifetimes, chemical stability, and the wide range of available emission wavelengths.

The main exception is blue-light emitters. The operational stability of organic emitters is crucial for practical applications, as emitters must maintain 95% of their initial brightness (T95) after 10,000 hours of operation [6]. In contrast, state-of-the-art blue G2 emitters exhibit a T80 lifespan of less than 160 hours [6], which is why G1 emitters are still exclusively used for blue light in commercial OLEDs. As a result, blue-light generation accounts for about 50% of the power consumption in devices like modern smartphone displays [7]. The widespread use of noble metals such as iridium and platinum raises concerns among both the OLED industry and academic communities. The scarcity and high cost of these metals, combined with their negative environmental impact, pose challenges to the sustainability and scalability of the OLED industry [8].

In response, recent years have seen the development of compounds capable of triplet harvesting without the need for heavy metals. These compounds, which exhibit thermally activated delayed fluorescence (TADF), have garnered significant attention since 2012 when the first efficient OLEDs using TADF emitters were demonstrated [9]. Often referred to as third-generation (G3) emitters, these materials are purely organic and metal-free. G3 emitters can harvest triplet excited states due to the proximity between their S1 and T1 energy levels. When the energy gap (ΔES1-T1) is smaller than about 0.12 eV, thermal energy at room temperature can raise the T1 state to the higher-lying S1 state through a process called reverse intersystem crossing (rISC). Combining G2 and G3 emitters could result in OLEDs with the highest possible efficiency and stability. Today, two additional generations of OLED materials have emerged.

The fourth generation (G4) involves combining G1 and G3 molecules, where excited states from G3 molecules are transferred to G1 molecules via Förster resonance energy transfer. This process, known as superfluorescence, enhances the efficiency of light emission. The fifth and latest generation (G5) consists of materials with inverted singlet-triplet states, allowing electrically excited triplet states to transition to the singlet state and emit light.

Another disadvantage is the high production costs of the OLED devices. During the device production stage the active light emitting organic components are usually processed using energy intensive and technologically complex vacuum deposition (sublimation) methods. To increase the competitiveness level of OLED devices the new light emitting materials need to be developed, which can be processed with inexpensive solution-based methods (spin-coating, ink-jet printing), while maintaining high efficiencies and chemical stability. At the moment this problem has not been completely solved and a considerable effort is made by research community in this direction. Recently Cu-based organic materials were used in the OLED. [10]

Our position

Laboratory of Organic Materials has a long-time experience in the investigation of original organic materials for application in an organic light emitting diode (OLED). One of the first steps is quantum chemical calculations to predict molecule applicability as efficient light emitting material with necessary semiconductor properties. The solution containing organic molecules is further investigated to determine the properties of the compounds themselves. Then, obtained thin films are studied.

The laboratory has expertise in the determination of both the optical and electrical properties of organic materials. Optical properties like photoluminescence spectrum, photoluminescence quantum yield, and fluorescence kinetics are essential to define possible organic compound applications in OLED [11].

Nevertheless, semiconductor properties are equally important. Therefore, the laboratory pays great attention to the investigation of energy structure and electrical properties of organic semiconductors [12].

Energy levels of the compounds have been studied by photoelectron emission spectroscopy (PES) and spectral dependence of intrinsic photoconductivity, which provides information about molecule ionization energy (IE). The second method gives a good estimation of the energy bandgap between IE and electron affinity (EA) energy [13]. Local trap states in the bandgap have been investigated by temperature modulated space charge limit current method. Charge carrier mobility has been obtained by Time of Flight (ToF) or Charge Carrier Extraction by Linearly Increasing Voltage (CELIV) techniques [14].

Obtaining complete information about a chemical compound can determine its potential use in the organic light emitting diode. So far, most activities have focused on the investigation of the organic compound. As the main group of compounds, molecular glasses with fluorescence, phosphorescence or thermally activated delayed fluorescence properties have been used. The laboratory has worked on light emitting organic ionic compounds [15] and has investigated carbene–metal–amide (CMA) type organic emitters for OLED[16-21].

Future activities

In the future, the activities related to the investigation of OLED will be broadened. Investigation of thin film morphology and intermixing of two thin films will be added in the research action. It will be linked to the performance and lifetime of the diode. Use of flexible substrate is one of the advantages of organic light-emitting diode, which should also be developed in the laboratory of organic material.

- Methods for preparation of OLED on flexible substrates

ITO-coated polyethylene terephthalate (PET) films fits for the preparation of a flexible organic light-emitting diode. Cleaning procedure of PET substrate will be developed to increase the wettability of organic compounds. A new type of chucks will be bought in order to perform layer deposition from solution by spin-coating method. Vacuum deposition system and measurement system will be adapted to flexible thin films. Also, new encapsulation methods will be used to maintain flexibility. At the beginning, 25×25 mm^2 will be used, and then they will be gradually increased to 50×50 cm^2. By developing the methods of depositing OLED on flexible substrate will further open new research directions of the laboratory and makes possible to broaden applications, like, wearable and biocompatible devices.

- Degradation mechanism investigation by ellipsometry

Investigation physicochemical properties of the interfaces, and their dependence on the deposition conditions and their role in the performance and degradation kinetics of organic electronic devices is very important. Interfaces between thin films of different organic materials and multilayer structures should be investigated to understand the interface contribution to interfacial transport of electrons and the degradation of OLEDs, and to explore the possibilities of interfacial tuning with the aim to improve the OLEDs performance. Advanced spectroscopic ellipsometry (SE) technique can be used to study layered polymer/molecular glass systems tailored to the parameters of the film deposition and post-deposition treatments and analyse in-situ the degradation kinetics of the OLEDs device under the thermal and electrical load. Investigating OLED degradation is crucial because it directly impacts the performance, lifespan, and reliability of OLED-based devices.

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LIGHT AMPLIFICATION AND ORGANIC SOLID-STATE LASERS

State of the art

Low-energy consumption light emitters having high energy conversion efficiency are essential for applications in fields like sensing and telecommunications. In particular, personalized medicine increasingly relies on low-cost test probes, such as Lab-on-a-Chip devices, which allow individuals to quickly obtain lab results and apply targeted treatments. One of the core mechanisms of these test probes is the detection of light variations—whether in spectrum or intensity. For such purposes, a small, highly efficient, and potentially wavelength-tunable light source is indispensable.

Organic solid-state lasers offer a promising solution because they are not only flexible and wavelength-tunable but can also be scaled to a few micrometers in size. These lasers can be integrated into both organic and inorganic photonic-integrated circuits, making them highly versatile for different applications. In the realm of telecommunications, especially for short-range communications, these lasers can be utilized within polymer fibers, with the telecommunications window operating in the near-infrared region. Organic solid-state lasers are particularly notable for their highly efficient energy conversion, especially in the infrared spectral range [1,2]. Organic compounds have long been used in dye lasers, and many of the same or similar compounds are now being utilized in organic solid-state lasers. These lasers use a wide variety of organic molecules, ranging from low molecular weight compounds to dendrimers and polymers.

The systems that exhibit the lowest amplified spontaneous emission (ASE) threshold values—below 1 μJ/cm^2—are typically dye-doped matrices [3,4]. Without a matrix, molecules are too closely packed, leading to significant intermolecular interactions that quench the excited states. This issue was partially mitigated by adding bulky side groups to dye molecules, but even then, the ASE threshold value remains an order of magnitude higher compared to guest-host systems [5,6]. ASE excitation energy also varies depending on the spectral range, with the smallest thresholds observed for blue emitters (below 1 μJ/cm^2) [3] and green emitters (similarly low thresholds) [4]. Yellow emitters have an ASE threshold of around 10 μJ/cm^2 [7], red emitters require about 24 μJ/cm^2 [8], and infrared emitters show thresholds of approximately 20 μJ/cm^2 [9]. These impressively low thresholds were achieved despite the photoluminescence quantum yield (PLQY) being below 25%. It stands to reason that even lower ASE thresholds could be attained if the PLQY were higher.

One promising avenue for enhancing the luminescence of organic materials is the incorporation of metallic nanoparticles (NPs) into the organic matrix. When placed in an electromagnetic field, properly excited metal nanoparticles can generate a plasmon field, which can, in turn, amplify the luminescence of surrounding organic molecules [10]. There are, however, numerous factors that influence the enhancement of luminescence, such as the shape, size, and dimensionality of the nanoparticles [11]. Other critical factors include the orientation of the dye dipole moments relative to the nanoparticle surface normal, the distance between the dye and the metal nanoparticles, the overlap of the plasmon resonance with the organic dye's absorption and emission bands, the radiative decay rate, and the quantum yield of the luminescent molecules themselves [12]. Luminescence can be significantly increased if the appropriate conditions are met within the metal NP-organic matrix. Among metallic nanoparticles, silver nanoparticles (Ag NPs) are particularly favored due to their exceptional physical, chemical, and biological properties. Ag NPs offer several advantages over other metallic nanoparticles: they exhibit minimal optical loss during surface plasmon propagation, are non-toxic, have excellent electrical and thermal conductivity, remain stable under ambient conditions, and are relatively low-cost compared to metals like gold or platinum. Additionally, silver nanoparticles possess a primitive structure and exhibit broad absorption of both visible and far-infrared light, further adding to their utility. Moreover, their chemical stability makes them even more appealing for practical applications [13]. Several studies have already demonstrated the potential of nanoparticles to enhance ASE efficiency. For instance, nanoparticles [14] and metal nanostructures [15,16] introduced into the gain media have been shown to reduce ASE threshold values by as much as tenfold. This reduction in the ASE threshold value is a significant advancement, opening the door to a new category of organic lasers: surface plasmon amplification by stimulated emission of radiation, or "spasers" [17].

Our position

Laboratory of Organic materials has started an investigation of light amplification in 2010. During this time, investigation method for a full description of the compounds has been established. Optical properties of solution containing organic molecules have been investigated to determine the further investigated compounds. Investigation of thin film deposition parameters is investigated afterwards. Emission spectra and photoluminescence quantum yield are one of the most important parameters which are studied in thin films. Light amplification properties are obtained via amplified spontaneous emission (ASE) by line method. Specific measurement set-up was made to measure ASE excitation threshold energy, light gain and losses coefficients. More than 100 compounds were investigated during this time in close collaboration with chemists. The investigated compounds emit light in the red and infrared spectral region. All investigated compounds were molecular glasses, and ASE properties were investigated in neat films or polymer matrix. Thin-film preparation from solution and reduced photoluminescence quenching are one of the advantages of molecular glasses.

One of the first works in the field of optical amplification systems was done in 2012, where amplified spontaneous emission of molecular glasses were investigated [19]. 4-(Dicyanomethylene)-2-methyl-6-(4-dimethylaminostyryl)-4H-pyran (DCM) red-emitting molecule has served as a base of all derivatives. Glass state of thin films was archived by adding bulky trityloxyethyl groups at the electron donor side of the molecule. The neat film of DCM does not exhibit fluorescence, but the photoluminescence quantum yield (PLQY) of the systems that we have prepared was up to 3% [20]. As a result, amplified spontaneous emission excitation energy as low as 90 J/cm2 was obtained. Further work was done to increase the synthesis yield of investigated compounds with a double increase in PLQY, but without significant changes in ASE excitation energy [21]. It was achieved by substituting methyl group with tert-butyl group (DWK-

1TB molecule). Several other modifications were done to electron donor and/or electron acceptor group to improve emission efficiency till DWK-1TB molecule was modified by changing malononitrile group as the electron acceptor to ethyl and one nitrogen group. These changes benefited in the optical properties of the neat thin film. PLQY increased up to 23%, while ASE threshold energy was decreased to 24 J/cm2 [8], which now is close to the best results for red emitters found in the literature. During the investigation of DCM derivatives, bis-DCM derivatives with the light emission in the near-infrared region were developed. The best performance of 170 J/cm2 ASE threshold energy with emission at 743 nm was obtained [22,23]. Recently we have applied active matrix in the gain media that consist of Alq3 derivatives to enhance the ASE efficiency [24].

Future activities

- Influence of metal nanoparticle surface plasmon resonance on ASE properties of organic materials

Regarding optical light amplification systems, the main goal will be the development of metal layer preparation protocol and selection of plasmonic design for optical amplification of light. For chemical metal nanoparticle synthesis, metal precursor, reducing agent, and stabilizing/capping agents are needed. Reducing agent concentration determines the size and shape of metal nanoparticles. Unprotected metal nanoparticles can easily agglomerate due to their small size; therefore, stabilizing is required. It allows obtaining a stable metal nanoparticle solution. Nanoparticles will be synthesised in aqueous solution, but organic material usually cannot be dissolved in water; therefore, metal nanoparticles will be transferred to an organic solution like chloroform or toluene afterwards. For this reason, reducing agent and stabilizing should be changed to one which can disperse nanoparticles in organic solution. The transfer can be made through a chemical reaction, centrifugation, and ultrasonic treatment. The size of nanoparticles will be tuned to match absorption and/or emission spectra of organic compounds. Synthesised nanoparticles will be mixed with laser dye or laser dyes deposited on the prepared metal nanostructure.

- Investigation of NIR emitters.

Organic compounds have been widely used in dye lasers and the same or similar compounds can be found in organic solid-state lasers. Most of the compounds have emission in the visible spectral region with the amplified spontaneous emission or laser emission excitation threshold energy below 1 $\mu J/cm^2$. Organic near infrared emitters have higher threshold energies, but they are more competitive compared to inorganic infrared lasers. Inorganic III-V semiconductor has low exciton binding energy (around 6 meV) which partially is the reason of low photoluminescence quantum yield of these materials. Additionally, a specific three or mostly a four-level system should be made to get population inversion. Organic materials exhibit the four-level energy system in the molecule and no additional modifications should be done. Organic compounds have higher Frenkel exciton binding energy (more than 200 meV), which increases the recombination possibility of the excitons. Organic materials that form thin films from solution would additionally benefit due to the possibility to make lasers by simple wet casting methods. Thus, such properties could increase the applications of lasers in telecommunication, bioimaging and lab-on-chip

Networking

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NOVEL MATERIALS FOR LUMINESCENCE DOSIMETRY

State of the art

Thermo- and optically-stimulated luminescence (TL and OSL) have been known and practically used in dosimetry for a long time. TL materials have been used in personnel, environmental and clinical dosimetry for many years. The main groups for dosimetric materials studied are fluorides (LiF:Mg,Ti; LiF:Mg, Cu,P; CaF_2:Mn; CaF2:Dy), sulphates ($CaSO_4$:Mn; $CaSO_4$:Dy: $CaSO_4$:Tm), borates ($Li_2B_4O_7$:Mn; $Li_2B_4O_7$:Cu), oxides (Al_2O_3:C; Al_2O_3:Mg,Y; BeO, MgO) and others. Among the prospective materials for the new clinical dosimetry and space exploration areas the nanopowdered materials and optical fibers with different dopants are being studied [1,2]. At present, standard commercially available dosimeters are used for the needs of most radiation fields (among them the highest-sensitive are LiF:Mg,Cu,P (TL) and Al_2O_3:C (OSL)), but in some areas there is still a demand for new materials with tailored properties. The need for new TL and OSL materials exists is limited to specific applications; any new material must satisfy the requirements for those applications. Therefore, there is a need to explore more sensitive materials that show linear TL responses over a wide range, materials that are energy independent, thermally stable and have low fading. Studies on **nanomaterials** have reported high sensitivity and saturation at very high doses. Therefore, they have potential application in dosimetry of ionizing radiations for measurements of high doses, at which conventional microcrystalline phosphors saturate [3].

Novel approaches under development in dosimetry

- Novel approaches under development include **dosimetry for medical needs**, such as two and three-dimensional dosimetry for radiotherapy applications, dosimetry for new radiotherapy modalities, such as laser-induced particle beams, FLASH radiotherapy, and magnetic resonance-guided radiotherapy. The safety and efficacy of novel theranostic agents, targeting increasingly complex targets, can be well served by comprehensive dosimetry. In this context, **artificial intelligence methods, especially machine learning and deep learning algorithms**, may play a crucial role. An overview of upcoming opportunities for integrating artificial intelligence methods into the field of dosimetry in nuclear medicine is given in [4].

- There is continuous demand for efficient TL dosimeters for monitoring **high-dose levels of swift heavy ion (SHI) radiation** used extensively in medical applications. Moreover, SHI-exposed phosphors can be used for high energy space dosimetry, ion beam dosimetry for personnel applications, radiotherapy, or diagnostic purposes, etc. Therefore, there is considerable scope for work on SHI dosimetry [5]
- The use of **personal neutron dosimetry** currently grows rapidly. Recently, $CaSO_4$:Dy and MgB_4O_7:Ce, Li [6]were synthesized to study neutron dosimetry. Moreover, materials containing Li, or Li and B simultaneously, were found to be more sensitive to neutrons. If these materials were enriched in ^{6}Li and B, isotopes became sensitive to thermal neutrons [5]. Therefore, future work may be focused on developing a thermoluminescent material sensitive to neutrons.
- Another prospective area of luminescence dosimetry is **OSL dosimetry for case of high energy physics (HEP)**. The main advantages of the OSL materials are: 1) a dynamic range that covers seven orders of magnitude; 2) a very high sensitivity (100 µGy). Application of the OSL method enables high spatial resolution 3D dose imaging [7].
- The main challenge for luminescence dosimetry is in **materials engineering**. Investigating and elucidating the roles and predominance of defect clustering and localized transitions in high-sensitivity TL/OSL materials may also play a key role towards a more guided "defect engineering" of new material. A better understanding of the influence of synthesis parameters and methods on the final luminescence and dosimetric properties is required [8,9].
- One of the most important and still actual aspects of TL and OSL application is **basic research of materials,** which together with photoluminescence, radioluminescence and photoluminescence excitation studies allows effective revealing of luminescence mechanisms in many fundamental problems. Different TLD materials in the form of glass, microcrystalline, nanocrystalline phosphors have been studied in search of new prospective TL/OSL materials. The search for new TL materials should aim for simplicity of glow curves, a high range of TL response linearity and very low fading. Furthermore, the TL mechanism is also very important and must be considered before developing new efficient materials for different applications. An example of such newly proposed dosimetric material is ZnO doped with transition metals and rare-earth elements [10].

Our position

Researchers of the dosimetry group from Laboratory of Spectroscopy and Laboratory of Optical Materials have a long-term experience in studies of dosimetric properties of various dielectric materials [11,12]. The main task of these investigations was elucidation of the luminescence mechanisms using TL/OSL methods and estimation of dosimetric properties suitable for practical application. The dosimetry group has a specific knowledge of in the field of luminescence processes and modern sophisticated equipment, such as Lexsyg Research TL/OSL reader (Freiberg Instruments) apart from other equipment for spectral measurements. At present the main direction of study is connected with luminescence and dosimetric properties of wide band dielectrics. TL/OSL investigation of wide band-gap dielectrics, including oxides single crystals, polycrystals, powders and ceramics, optical glass fibres will give new insights in luminescence mechanisms and estimate applicability of new materials for dosimetry of ionising and UV radiation in the fields of medicine, radiation safety, environment, industry and space flights.

Recent studies in the luminescence dosimetry field concerns the following materials:

- **Al_2O_3 (alumina)**–based dosimetry materials. The best known and widely used dosimeter material on alumina basis is carbon-doped aluminium oxide Al_2O_3:C (TLD-500) ($E_g > 6$ eV), used as highly sensitive TL, and OSL material for personal dosimetry. However, as a personal dosimeter, Al_2O_3:C is useful only in the dose range 10 µGy–10 Gy and is not suitable at higher doses. Efforts were undertaken to find other alumina-based dosimeter materials using different dopants. It was shown by us [13], that only for α phase Al_2O_3 Cr^{3+} ions give the well-pronounced luminescence bands around 690 nm in TL emission spectra. Our data, e.g. ref. [11, 14] indicate that dosimetric properties of Al_2O_3 the form of ceramics from nanopowder produced by means of nanotechnology, can possess such advantages as high sensitivity to ionizing radiation, uniform distribution of luminescence centres, appropriateness to high radiation doses and low price compared to corresponding single crystals. In future we plan the investigation of the material using mainly the OSL method.

- **AlN (aluminum nitride)** has been previously studied by us for TL and OSL applications [12]. It has a number of advantages compared to Al_2O_3, a much higher sensitivity to ionizing radiation and in particular to UV radiation [12], a wider linear dynamic range, lesser dependence of TL response on the readout (heating) rate. However, on the negative side, it has much higher signal fading rate at room temperature. We have assigned the fading to tunnel recombination process between donor–acceptor pairs. Our ideas to diminish the detrimental fading phenomenon include creating deep traps by additional doping of AlN with transition metals and rare earth ions. AlN ceramics samples, pure and doped with Y_2O_3, Eu_2O_3 and GaN were studied for photoelectric effect, photoluminescence spectra and kinetics and thermoluminescence under irradiation with UV light from above- and below- bandgap spectral region [15, 16]. Properties of pure and Eu and Mn doped AlN were also studied recently [17,18] The additional studies of materials are planned using mainly the OSL method.
- **Wide band gap dielectrics,** on the example of $LiGaO_2$ (LGO). LGO is a wide band gap (E_g=5.6-6 eV) wurtzite-structure crystal, relatively recently proposed for TL/OSL dosimetry with Cu+ as dopant. Our study of nominally pure $LiGaO_2$ crystal [19] has shown that UV light irradiation of this material produces complicated recombination processes, which are followed by TL and OSL. The further investigations have shown that, although this material provides only a weak response to ionising radiation and UV light and hardly can be applied as a dosimetric material, the TL/OSL methods used are very useful instruments for elucidation of the energy transfer and luminescence mechanisms, which allows revealing and characterization of pyroelectrical luminescence in LGO [19,20].

The planned experimental study is relatively well-supported by the existing infrastructure. In year 2020 due to the ISSP UL Infrastructure project, a new, state-of-the-art experimental dosimetric system was obtained, Lexsyg Research TL/OSL reader (Freiberg Instruments, Germany), which enables TL and OSL measurements after X-ray and beta-ray irradiation. Its capabilities are further enhanced by a self-made accessory, allowing an additional sample irradiation UV light. In 2024 the device was upgraded with a Peltier module, enabling TL/OSL measurements at temperatures below RT, beginning from -50 C. The TL, OSL and radioluminescence signals can be spectrally analysed using an additional spectrometer and CCD camera. Development of the OSL experimental setup is planned using LED sources of different wavelengths. Additionally, the dosimetric studies are complemented by photoluminescence emission and excitation spectra measurements. Therefore, there is a need to enhance the experimental basis for the PL/TL spectral measurements by acquisition of Andor Spectrograph Kymera with 4 gratings, with ICCD IStar 320 and accessories), and closed cycle cryostat (5.5- 800 K) for optical spectroscopy.

Future activities

- **TL investigation of wide band-gap dielectrics**, including oxides single crystals, polycrystals, powders and ceramics, optical glass fibres for application in medicine, radiation safety, environment, industry, space flights placing the main emphasis on material study for UV light dosimetry. Dosimetric properties of Al_2O_3, AlN, ZnO doped with transition metal and rare earth elements will be studied in order to find out the optimal doping conditions, providing high sensitivity, large dynamic range and low fading rate of the stored signal.

- Further **development of the OSL method** basing on the available Lexsyg TL/OSL reader. Study of the OSL materials mainly based on the doped Al_2O_3 and AlN ceramics and related materials. OSL materials are especially useful for use in the portable devises for the field measurements, however, special precautions must be undertaken to prevent the optical bleaching by the ambient light.

- TL/OSL methods have **a fundamental role in research on luminescent materials**, including scintillators and persistent phosphors. TL is extremely sensitive to small concentrations of defects and will be used to detect defect energy levels or to investigate phenomena such as tunnelling between defects. This will help to engineer new luminescent materials for a variety of application.

- Future development of the TL/OSL measurement equipment is planned in the following directions: - upgrade of the Lexsyg research TL/OSL reader for irradiation with a UV light source (UV lasers, Deuterium lamp), using the optical lightguides; - upgrade of the Lexsyg research TL/OSL reader software; - development of the OSL experimental setup using LED sources of different wavelengths; -upgrade of the set-up for PL/TL spectral measurements with a new spectrograph and CCD camera.

Networking

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ELECTRONIC PROCESSES AND CHARGE TRANSFER MECHANISMS IN LUMINESCENT MATERIALS

State of the art

The exploration of luminescent materials with band gaps exceeding 3 eV is becoming increasingly vital due to their broad range of potential applications across diverse technological fields, including optoelectronic devices, sensors, bioimaging, and environmental monitoring. [1] Research in this domain has expanded to cover various facets, including the development of luminescent centers—both intrinsic and extrinsic (doping-induced)—and the in-depth understanding of the electronic processes, charge carrier dynamics, and relaxation mechanisms involved in luminescence. [2,3]

Recent technological advances have fuelled a growing interest in two promising classes of luminescent materials: mechanoluminescent and electroluminescent materials. Mechanoluminescence, the phenomenon in which mechanical stress induces light emission, has garnered considerable attention for its potential in applications such as stress mapping, wearable sensors, and smart materials.[4] Recent studies have focused on improving the sensitivity and stability of these materials, as well as developing new mechanoluminescent compounds that can operate under wider range of mechanical conditions.[5, 6]

Electroluminescent materials, which emit light in response to an applied electric field, are another area of rapid development. These materials are key components in devices such as light-emitting diodes (LEDs), flat-panel displays, and electroluminescent sensors.[7] Research efforts are now focused on developing new electroluminescent compounds that are both environmentally friendly and cost-effective, with particular emphasis on flexible and transparent devices that could revolutionize display technology and wearable electronics.[8,9]

Another promising area of research is the intersection of luminescent materials and additive manufacturing. Additive manufacturing, or 3D printing, offers unique opportunities to create complex, customizable structures with embedded luminescent properties. By incorporating luminescent materials directly into 3D-printed components, it is possible to create multifunctional devices with integrated sensing, lighting, or signalling capabilities.[10] Recent studies have explored methods to enhance the printability, stability, and performance of luminescent materials for these applications, with promising results.[11,12]

One of the key challenges in the development of new luminescent materials is the need to better understand and control the underlying mechanisms of luminescence, including charge carrier dynamics and defect engineering. Advanced characterization techniques, such as time-resolved photoluminescence spectroscopy, thermoluminescence analysis, and synchrotron-based methods, are increasingly being used to study these processes at the atomic level.

Our position

Significant work is invested world-wide in studies of long-lasting (persistent) luminescence of solids. While this phenomenon is the basis of numerous applications (visualization in darkness, various indicators, traffic signs etc.), the underlying fundamental mechanisms providing the ultra-long luminescence decay time are not clearly understood.

The study of these materials has seen a surge in recent years. The Optical Materials Laboratory and the Laboratory of Spectroscopy have made strides in developing materials that exhibit photoinduced long-lasting luminescence, an effect with considerable implications for applications such as emergency lighting, medical diagnostics, and environmental sensing.[13-22]

The team within the Optical Materials Laboratory has performed a series of in-depth studies of electronic processes in long-lasting luminescence materials [13]; a new mechanism of long-lasting luminescence involving electron tunnelling has been proposed.[21] The work of this and other international groups on mechanisms of long-lasting luminescence mechanisms is summarized in our topical review paper.[20]

Additionally, mechanoluminescence is extensively studied combining the previous knowledge on the electronic processes in persistent luminescence materials with the newly developed experimental setup for mechanoluminescence tests. Studies on various production methods, host materials and spectroscopic properties are performed with a row of publications in the making.

Not only the experimental setup for mechanoluminescence measurements was published in detail in year 2022 [15], but also a completely new data analysis protocol was developed and published for automated 2d image analysis of mechanoluminescence while the parts are deformed.[16] This allows the use of our developed materals to be used in a form of paint for real practical applicaitons.

Our laboratory is also exploring luminescent glass and translucent ceramics to enhance materials with unique optical properties [22], as it proposed also in monograph by Kitai, A [23].

In scintillator/dosimetry field, the radio- and photoluminescence studies of prospective scintillator ZnO:In and ZnO:Ga were conducted. The results of experiments show an extremely fast subnanosecond decay of near-band-edge luminescence. [19]The time constant determined for the decay of this luminescence was ≈17 ps [18] and it is very close to the present best result 15 ps found by Yamanoi K. et al. [24].

Thermostimulated luminescence investigation of Al_2O_3:C layer on metallic aluminium was conducted [17] and it was shown that the charge traps in Al_2O_3:C layer are similar to those known in the widely used thermoluminescent dosimeter TLD – 500. An understanding of the electronic processes in these layers is necessary to develop radiation-detecting 2D screens.

Thermostimulated luminescence analysis of oxygen vacancies in HfO_2 nanoparticles is provided [25].

Future activities

For persistent luminescence materials:

The studies of the impact of spatial distribution of donor-acceptor pairs on persistent luminescence are planned. The cooperation between Povdiv University (Bulgaria) and Optical Materials laboratory is ongoing in the subject of **luminescent, phone readable anti-counterfeiting tag**s. Also, different **persistent luminescent glasses** are being studied and will be in the focus in the future.

For the **scintillator** field, two main directions are foreseen for ZnO based scintillator materials:

- to elucidate the main mechanism(s) contributing to room temperature luminescence;
- to find a more efficient donor and its optimal concentration in ZnO for an efficient suppression of charge carrier trapping at intrinsic defects.

In addition, the knowledge on alumina-based dosimetry is applied to create dosimetric coatings using Plasma Electrolytic Oxidation. With efforts to produce alumina coatings on metal surface, the research can not only lead to the creation of a very promising method and material for practical applications, but also give an insight on alumina ceramic behavior under ionizing radiation.

The work on **mechanoluminescence will be continued further**, as initial feedback from companies working with additive manufacturing methods (Baltic 3D) was very positive, and the possibilities for joint projects or commercialization are outlined.

In future activities, one of the key focal points will be **the automated synthesis of complex oxide materials optimized for optical applications**. This will include leveraging advanced methods such as Plasma Electrolytic Oxidation (PEO), which has proven to be highly effective in generating oxide coatings with tailored properties, including enhanced luminescent and optical characteristics.

In addition to PEO, **other advanced synthesis techniques will also be explored to optimize the performance of complex oxides**. These may include sol-gel processing, hydrothermal synthesis, and combustion methods, all of which offer unique advantages for producing fine-tuned luminescent materials with well-defined structures and morphologies. By automating these synthesis processes, it will be possible to accelerate the development and discovery of new materials by enabling high-throughput screening of different compositional and structural parameters.

Future work will also focus on the **integration of machine learning algorithms to assist in the optimization of synthesis parameters**, thereby speeding up the discovery of high-performance materials.

In addition, one of the focuses of the lab **is finding new applications with higher TRL for developed scientific concepts and ideas through tight collaboration with industry**. One of the successful higher TRL applications of optical phenomena is in-situ water quality measurement device that uses optical spectroscopy developed in the Optical Materials laboratory – Spectromarine.com. A new collaboration network was opened, including participation in "Water Europe" (https://watereurope.eu) - European platform that promotes innovation, research, and sustainable water management practices.

Networking

Abroad

- Bulgaria, Plovdiv University, Bulgarian Academy of Sciences, Prof. T. Eftiimov
- Germany, GSI Helmholtzzentrum für Schwerionnenforschung, Dr. P. Boutachkov
- Finland, Tampere University and University of Turku, Dr. V. Lahty, Dr. M. Lastusaari
- Czech Republic, Institute of Physics AS, Dr. P. Bohacek and Dr. M. Nikl
- Estonia, Institute of Physics, University of Tartu, Dr. S. Zazubovich and Dr. A. Krasnikov

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X-RAY ABSORPTION SPECTROSCOPY USING SYNCHROTRON LIGHTSOURCES

State of the art

The structure of materials determines their properties, making its understanding and control vital for practical applications. X-ray absorption spectroscopy (XAS) with synchrotron radiation is a powerful tool for probing local atomic and electronic structures in solids, liquids, and gases [1]. It can be used to study crystalline, nanocrystalline, and disordered solids as well as liquids and gases. XAS is a well-established but evolving method, closely linked to advances in synchrotron facilities. Nowadays, there are about 50 active synchrotron facilities around the world, and 17 of them are located in the EU Member States. The European Strategy Forum on Research Infrastructures (ESFRI) Roadmap 2021 outlines the strategic vision for the development of Europe's large-scale research facilities.

During the last ten years, there has been continuous growth in the number of publications (according to the WoS database) on the development and application of XAS, now reaching approximately 3,000 papers per year. XAS is a multidisciplinary field of research that includes studies of materials and their transformations in material science, physics, chemistry, life sciences, environmental sciences, cultural heritage, and medicine. The technique provides a wide range of opportunities for *in-situ* and *operando* studies, which were recently reviewed in [1]. The theoretical foundation of X-ray absorption spectra is based on Fermi's Golden Rule, and the spectra are typically computed numerically using multiple-scattering theory [2]. Structural information is encoded in the extended X-ray absorption fine structure (EXAFS). Retrieving it from experimentally measured spectra requires significant effort and can be challenging [3, 4]. Therefore, the development of methodologies for the analysis of X-ray absorption spectra, based on advanced numerical methods [4], including machine learning methods [5], is a hot topic in current research, actively pursued at ISSP.

Recent advances in machine learning and Big Data now enable autonomous experimentation, allowing automatic control of operando parameters and real-time data processing [6], which enhances experimental throughput, and reliability and supports new methodologies.

New X-ray and extreme ultraviolet sources like free-electron lasers (FELs) offer insights into dynamic molecular structures and fundamental photophysical, photochemical, and biological events, as well as coupled electronic and nuclear dynamics. Pump-probe experiments, combining synchronized pulsed laser excitation with X-ray pulses, enable a new time-domain view of electron correlations, with implications for designing molecules and materials with tailored functions [7].

Our position

The EXAFS Spectroscopy Laboratory is one of the world's leading groups in developing and applying advanced methodologies for the analysis of X-ray absorption spectra, including approaches based on regularization technique, atomistic simulations such as molecular dynamics and reverse Monte Carlo (RMC) modelling, and machine learning methods. The Laboratory has world-class expertise in the use of synchrotron radiation X-ray absorption spectroscopy, an analytical tool for studying the local atomic and electronic structure of materials.

A set of leading ab initio (full-) multiple-scattering XANES/EXAFS software codes from the partners provides a solid foundation for experimental data analysis at ISSP UL. The use of theoretical simulations is supported by a high-performance computing (HPC) infrastructure (Linux Cluster) with a theoretical peak performance of about 150 teraflops. This enables ISSP UL researchers to fully exploit the potential of XAS, allowing for the incorporation of both static and thermal disorder into structural models. As a result, new possibilities are opened for investigating structure-property relationships in emerging materials.

The research at ISSP UL includes but is not limited to various functional nanomaterials, thermochromic and photochromic materials, compositionally complex materials, as well as disordered materials (thin films, glasses, etc.). Over the past 10 years, more than 40 projects have been conducted at synchrotrons such as PETRA-III (Hamburg), MaxIV (Lund), SOLEIL (Paris), ELETTRA (Trieste), ALBA (Barcelona), and ESRF (Grenoble), resulting in over 130 peer-reviewed publications. The results of these experimental projects have contributed to the implementation of 18 international and national research projects, 12 of which are directly related to the use of the XAS method. The high quality of the laboratory's research is highlighted by the inclusion of its recent results in the *Highlights 2018-2019* of the ELETTRA synchrotron center, *Highlights 2021* of the ESRF synchrotron facility, and *Highlights 2022* of the MaxIV synchrotron center. In 2024, the laboratory contributed two chapters to the latest volume of the International Tables for Crystallography, dedicated to X-ray absorption spectroscopy and related techniques [1], as well as a chapter on X-ray absorption spectroscopy in high-entropy material research in a recent book [8]. The Lab's work on the study of the structure-property relationship in the versatile copper molybdates was included in the Latvian Academy of Sciences YearBook 2022. The laboratory represents Latvia in the European Synchrotron and Free Electron Laser User Organisation (ESUO) and in the International X-ray Absorption Society (IXAS).

In addition to carrying out its own projects, the laboratory provides consulting services to research groups worldwide on EXAFS data analysis and interpretation. This activity is growing due to the increasing reputation of the group and the popularity of the EXAFS method and is likely to significantly expand the scope of cooperation and open up new opportunities in the future.

Several groups around the world have been active in advanced XAS data analysis for a long time and can be considered "competitors". The group from Wigner Research Centre for Physics (Hungary) is the ancestor of the RMC method and is developing it mainly for application to disordered materials such as solutions and glasses. Another group from Camerino University (Italy) is the main developer of the GNXAS code for ab initio XAS simulations but provides also an RMC part dedicated to disordered materials. An international group, including teams from ISIS, the University of Cambridge, the University of Oxford, Queen Mary University of London (UK), and NIST (USA), is involved in the development of the reverse Monte Carlo method for the simultaneous analysis of various data types (neutron & X-ray total scattering & the Bragg profile, EXAFS, single-crystal diffuse scattering). Currently, there are only a few major players in the field of machine learning applications for XAS - Fritz Haber Institute of the Max Planck Society (Germany) and Brookhaven National Laboratory (USA) - but this number is expected to grow soon due to the method's potential. Meanwhile, several groups (e.g. from Sapienza University of Rome (Italy)) working in the fields of liquids and disordered compounds use molecular dynamics to simulate the configuration-averaged XAS spectra.

Future activities

The EXAFS Spectroscopy Laboratory will align its future research with European research trends outlined by the European Strategy Forum on Research Infrastructures ESFRI, utilizing large European synchrotron facilities that served over 24,000 users in 2017. The lab is open to collaborations within the EC Horizon Europe program and other research initiatives.

The main research directions will involve the development of novel methodologies based on machine learning methods and their application to the study of high-entropy materials, energy, and smart materials.

Rising energy consumption and limited resources are key challenges. The EXAFS Spectroscopy Laboratory is studying oxide dispersion strengthened (ODS) alloys, crucial for nuclear fusion energy production, and advancing Europe's role in nuclear fusion technology through the EUROfusion project. Additionally, the lab will continue exploring multifunctional materials for X-ray sensing, thermochromic, electrochromic, photocatalytic, thermoelectric, and other energy applications [9, 10, 11].

Materials science under extreme conditions, such as ultra-high pressures and temperatures, offers a path to discovering new materials not possible with conventional methods. These conditions are created using tools like diamond anvil cells (DACs). Combined with theoretical structure prediction tools based on ab initio quantum chemistry, such experiments accelerate materials discovery and enhance understanding of their properties. The EXAFS Spectroscopy Laboratory collaborates with synchrotron centers at SOLEIL (Paris) and ESRF (Grenoble) on these studies [12].

Key challenges in information technologies include the growing demand for storage capacity, computing speed, smart sensors, and energy-efficient solutions. The EXAFS method, combined with advanced analysis methods and ab initio simulations, will be an invaluable tool for future in-situ and operando studies of emerging materials (e.g., 2D van der Waals and core/shell nanostructures, thin-film thermoelectric and photochromic materials, hybrid organic-inorganic systems) [9, 10, 13, 14]. Mastering advanced experimental techniques will contribute to understanding these materials and promoting their future application. These efforts will be carried out in close collaboration with groups at DESY as part of the PETRA-III storage ring upgrade program.

The new direction of our research aims to enhance the understanding of multicomponent alloys, also known as high entropy alloys (HEAs) or complex concentrated alloys (CCAs) [8]. HEAs exhibit superior mechanical, oxidation, corrosion, and irradiation properties compared to commercial alloys due to five key effects: high-entropy effect, severe lattice distortion, sluggish diffusion, short-range order effect, and "cocktail" effect [8]. Understanding these phenomena in both homogeneous and heterogeneous HEAs at the atomic level requires detailed knowledge of the composition dependence of short-range order, which can be probed by XAS combined with advanced atomistic simulations [15, 16].

Developing EXAFS data analysis methods is a key focus at ISSP. The next breakthrough will likely come from applying machine learning, enabling faster material simulations, decision-making, and real-time experiment control. This will improve efficiency at synchrotron facilities and create new possibilities. The laboratory plans to advance this technology through its involvement in two COST Action CA22143 and CA22154.

The sustainability strategy of the laboratory is based on four main activities: 1) the continuous search for and involvement of students and postdoctoral researchers; 2) the continuous improvement and development of team potential and available resources through in-lab seminars and discussions, and international schools/workshops/conferences; 3) the participation of young researchers in synchrotron experiments; and 4) collaboration with key players in the field to maintain and enhance the team's competitiveness.

The EXAFS Spectroscopy Laboratory team has developed several demonstrators realized as software packages for EXAFS data analysis, which are available to the international community on the lab's website. These packages are also used for teaching purposes at international schools. Locally, the EXAFS Spectroscopy Laboratory is involved in the teaching process at the University of Latvia providing an MSc course (64 hours) "Microscopy and Spectroscopy Characterization Methods".

Networking

The EXAFS Spectroscopy Laboratory at ISSP UL currently offers consulting services to research groups worldwide on EXAFS data analysis and interpretation. This activity is expanding due to the growing popularity of the EXAFS method and the increasing number of synchrotron centers globally. In 2024, the laboratory organized the International Workshop on Recent Advances and Future Trends in EXAFS Spectroscopy (June 13-14, 2024, Riga, Latvia) and participated in organizing the COST EuMINe 1st General Meeting and Workshop (April 10-12, Bologna, Italy).

Collaboration with the high-tech industry is primarily feasible through long-term projects due to the specificity of the XAS method. However, short-term consulting services can be provided in particular cases.

Abroad:

- Germany: Helmholtz-Zentrum Berlin für Materialien und Energie (HZB), Dr. A. Smekhova.

- Germany: Deutsches Elektronen-Synchrotron—A Research Centre of the Helmholtz Association, Dr. E. Welter.
- Germany: Karlsruhe Institute of Technology, Dr. C. Bonnekoh, Prof. B. Gorr.
- Portugal: Centre of Physics, University of Minho, Prof. C. J. Tavares.
- Finland: Center for X-ray Spectroscopy, University of Helsinki, Dr. R. Bes.

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NOVEL LEAD-FREE AND LOW-DIMENSIONAL FERROELECTRIC MATERIALS

State of the Art

Ferroelectricity, discovered over a century ago, for a long time focused on lead-based perovskites. These materials, including lead zirconate titanate (PZT), have been crucial in technologies such as non-volatile memories, piezoactuators, ultrasonic transducers, and electro-optic devices due to their switchable polarization and piezoelectricity [1–2]. However, environmental and health concerns about lead, especially in biomedical applications, have spurred the search for sustainable, lead-free alternatives [3].

Among the most promising lead-free materials is $Na_{0.5}Bi_{0.5}TiO_3$ (NBT). NBT and its solid solutions have demonstrated comparable or superior performance to PZT in certain applications, such as ultrasound transducers [4]. Despite advances, challenges remain in the production process, leading to inconsistent results. Key issues include deviations from stoichiometry, grain growth, which affect stability of ferroelectric state and nature of electrical conductivity [5-7].

Chemical heterogeneity in the form of core-shell structures can be realized in NBT-based ceramics [8]. Presence of shells influences microstructure of ceramics and can have high impact on electric and ferroelectric properties of material [9].

Recent trends emphasize the miniaturization of ferroelectric materials into low-dimensional forms like nanopowders, nanofibers, thin films, and nanostructures. These materials often show enhanced properties at smaller scales and are used in ferroelectric diodes, negative capacitance devices, and microelectromechanical systems (MEMS) [10–13]. Memory and capacitor technologies remain dominant applications [11–13].

The exploration of 2D ferroelectricity has gained momentum with discoveries in van der Waals (vdW) materials and doped fluorites like $HfZrO_2$ [14]. Layered ferroelectrics, including $CuInP_2S_6$ (CIPS), show promise due to their ferrielectric ordering and ionic conductivity [15, 16]. Recent advancements in CIPS have revealed spontaneous polarization switching in ultra-thin samples, paving the way for new memory and switching devices [16, 17]. Current research is focused on integrating CIPS into functional elements like ferroelectric tunnel junctions and heterostructures [18, 19].

The electrocaloric effect (ECE) offers potential for cooling applications in microelectronics and environmentally friendly refrigeration. Despite extensive research, working cooling prototypes are rare due to inconsistencies in results, mostly originating from application of the indirect ECE determination method, the fact that the most promising results are obtained in thin films, which have low heat capacity, and also limited understanding of the nature of ECE and polarization at high electric fields [20]. Recent work has highlighted the need for new materials and methods, with multilayers of $Ba(Ti,Zr)O_3$ solid solutions showing ΔT values of up to 6°C [21]. Advancements in thick films and multilayers aim to balance high ΔT values with reduced device voltage [22, 23].

NBT-based materials, while trailing PZT in piezoelectric coefficients, exhibit high mechanical quality factors and large field-induced strains [6]. Expanding composition ranges and addressing challenges such as hysteresis could optimize these materials for various electromechanical applications [24]. Piezoelectric micromachined ultrasound transducers (PMUTs), with advantages over traditional PZT transducers, are being explored for biocompatible and medical uses [25].

Unconventional materials like ceria have shown giant induced piezoelectric effects, though currently practical only at low frequencies [26]. Research continues to improve frequency response and broaden applicability. Additionally, sustainable, lead-free ferroelectrics, including CIPS, are being developed for biomedical applications due to their multifunctionality and biocompatibility [27]. Partial atomic substitution in CIPS has been shown to enhance polarization and piezoelectric properties [28], though challenges in nanoscale characterization and understanding ionic conductivity remain.

Our Position

The Ferroelectric Materials Group, Laboratory of Optical Materials has extensive experience in ferroelectric ceramics, with a recent focus on lead-free materials like $Na_{0.5}Bi_{0.5}TiO_3$ (NBT). Our research has clarified misconceptions about Bi deficiency during sintering, showing that NBT remains stable with stoichiometric deviations [29–31]. We have also explored the electrocaloric effect (ECE) in NBT-BT-based solid solutions, conducting ECE experiments at fields up to 100 kV/cm to explore their cooling potential [32, 33], as well as characterized dielectric properties and field-induced strains in these materials [34].

Additionally, our research on Erbium (Er) luminescence has provided insights into the impact of disorder in the A-sublattice and electric field modulation of luminescence intensity [35]. We have developed lead-free piezoelectric micromachined ultrasound transducers (PMUTs) and explored environmentally friendly production methods for free-standing films, including $0.9NBT\text{-}0.1Sr_{0.7}Bi_{0.2}TiO_3$ thick films [36].

Our recent expansion includes advanced low-dimensional ferroelectric materials. Prof. Andrei Kholkin has joined our team in the role of ERA Chair, bringing expertise in Scanning Probe Microscopy and low-dimensional ferroelectrics. His knowledge in strain engineering and phase transitions complements our research, enhancing our work on nanodevices for energy conversion and biomedical applications [37–40].

Future Activities

Future research will focus on advancing lead-free and low-dimensional ferroelectric materials, developing production technologies, and expanding applications in energy harvesting, sensing, and cooling devices. Discovering new lead-free compositions and optimizing methods for bulk materials, free-standing thick films, low-dimensional piezoelectrics and multiferroics, including biological polymers, will be prioritized. Future activities will include:

- Further development of NBT and BT-based materials for actuators, sensors, transducers and electrocaloric devices;
- Study of dependence of core-shell structure in NBT-based compositions on composition and sintering parameters of the ceramics, revealing mechanism, responsible for its realization. Analysis of influence of core-shell structure on physical properties (impedance, domain structure, resistance to electrical breakdown, and fatigue).
- Development of producing technology of free-standing thick films via aqueous tape-casting for electrocaloric cooling [32, 33]. Research will also focus on microwave-assisted hydrothermal synthesis for NBT nanopowders with varying morphologies, essential for producing textured films [26].
- Development of novel functional ferroelectrics and low-dimensional structures for flexible sensors, and energy harvesting. Study of zero-, one-, and two-dimensional ferroelectrics, such as $CuInP_2S_6$ thin films and nanoflakes, aiming to optimize polarization switching and piezoelectric properties. Advanced nanoscale analysis will map functional properties and explore the interplay between polarization, strain, and surface chemistry. Special attention will be given to biological polymers.
- The research will target high electric field behaviors, optimizing piezoelectric coefficients, by electric field-induced mechanical strains, and fatigue resistance. For electrocaloric applications, it is aimed to achieve ΔT values of 5°C and above, enhancing the applied field range.

These research initiatives will drive advancements in both high-tech and biomedical sectors while promoting innovation in eco-friendly, lead-free ferroelectrics. Ultimately, the work aims to pave the way for sustainable applications across diverse fields.

Networking

Abroad:

- Lithuania, Vilnius University, Faculty of Physics, Prof. J. Banys;
- Germany, University of Duisburg-Essen, Institute for Materials Science and Center for Nanointegration, Dr. V. Shvartsman;
- Germany, Fraunhofer institute, Institute of Ceramic technologies and Systems, Dr. S. Gebhard;
- Switzerland, EPFL, Laboratory for in situ Nanomaterials Characterization with Electrons (INE), Prof. V. Tileli;
- Denmark, Technical University of Denmark (DTU), Dr. Milica Vasiljevic;
- France, University of Picardy Jules Verne, Dr. Abdelilah Lahmar;
- France, European Union, Piezoinstitute, the European Institute of Piezoelectric Materials and Devices – hub of European expertise and resources on piezoelectric materials and their applications, (ISSP UL participates in this organisation), piezoinstitute.univ-tours.fr.
- Taiwan, National Cheng Kung University, Department of Electrical Engineering, Prof. Chih-Hsien Huang;

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PERSISTENT LUMINESCENCE MATERIALS

State of the art

The persistent luminescence (PersL) is light emission lasting from seconds to many hours after ceasing of excitation source. The PersL solid state materials can store the energy of light or X-rays in advance and release it in a long-lasting afterglow emission. This is a valuable characteristic, for applications in different fields, with biomedicine as one of the most important. Recently, the PersL materials have found applications in biomedicine as biosensors, biomarkers, for background-free bio-imaging compounds, targeted drug delivery, diagnostics tools etc. [1-3, and Refs. therein]. For successful use in biomedicine, the solid state PersL materials must meet several main requirements:

- Material must be with very low toxicity.
- The dimensions of material particles must be small, preferably nanosized (≤ 200 nm).
- The particles must be reasonably stable in body fluids and be able to target the specific cells.
- Luminescence spectrum of the material must match up to the spectral region with relatively low absorbance for the main types of human tissues. It covers the spectral region of red and infra-red (IR) light, beginning from ~600 nm and lasting up to 1500 nm.

Presently, there are a lot of solid-state PresL materials with use cases in biomedicine [1-3, and Refs. therein]. The most important of them can be divided into several main groups:

- single and complex metal oxides doped with lanthanide group elements (Eu, Er, Dy, etc.) or transition group metal ions (Mn, Cr, Fe, etc.) [5-7];
- materials containing quantum dots [8],
- carbon nanomaterials [9].

For biomedical applications, all these materials demonstrate several favorable characteristics together with various imperfections. Unfortunately, most doped oxides, which form the dominant class of used biomaterials, are also potentially toxic to living cells [7], but materials with quantum dots and carbon nanomaterials are highly toxic [8, 9]. The facts above highlight existing problems and stimulate elaboration of new prospective red-infrared light emitting PersL materials with advanced qualities for biomedical use.

One of the actual fields for PersL material application is cancer cells identification in its early stages. Among many types of cancer, skin cancer/melanoma is one of the deadliest. Detection of skin cancer in its early stage is essential for patient survival. Usually, the patient's first contact is with a family doctor who is not a specialist in skin diseases. There are special forms of cancer such the Amelanotic Malignant Melanoma [10], which are not visually noticeable under normal circumstances. If activated PersL particles were injected into the skin of such a patient, it would allow visualization of cancerous tissue. In this case the new PersL materials emitting red light from the spectral region 600-700 nm, which is visible to the human eye, are promising.

Our position

The aim of our current research is the development of new solid-state material particles for use as markers and drug carriers in biomedicine. In particular, our research focusses on red/infrared (NIR) light emitting persistent luminophores. These materials hold promise for use in bio-imaging applications, both *in vitro* and *in vivo*, by enabling non-invasive visualization of tissues within living organisms as well as theranostics. Our current research has been done on several material groups.

The first group includes doped AlN materials. In the period from 2020 to 2023 years we have comprehensively studied luminescence processes in doped AlN ceramics and nanomaterials [11-14]. It was found that AlN:Mn possesses a number of characteristics, which could be prospective for bio-imaging. The material:

- may be synthesized in the form of nanoparticles,
- exhibits red 600 nm emission, possessing long-lasting PersL properties [14].

Nevertheless, it was also observed that the intensity of 600 nm luminescence for nanomaterials is much lower than that of ceramics. Additionally, the AlN nanoparticles readily degrade in water and leave behind aluminum ions, which are known to be harmful. The latter reduces the applicability of the AlN materials in biomedicine.

The second group of promising materials consists of doped calcium/magnesium carbonates and phosphates [15-18]. We are currently studying the materials of this group. These materials possess high biocompatibility and biodegradability [15]. Some of them are already in use for biomedical applications – for delivering drugs and imaging compounds to certain cells in the body [15 and Refs. therein]. For example, calcium phosphate particles functionalized with fluorescing cyanine dye have been used for bio-imaging [15]. At the same time, the PersL emitting nano particles, based on the doped host materials, have not been sufficiently studied.

Our research has shown that these materials:

- may be synthesized in the form of nanoparticles,
- exhibit red 600 nm emission, possessing long-lasting PersL properties and
- easily dissociate into nontoxic substances.

For this reason, we are currently further researching these particles for their biomedical applicability.

The third group of the materials includes the Mn-doped complex oxide $Mg_2Si_{0,1}Ge_{0,9}O_4$ (MSGO) for development of red light emitting PersL material, applicable for injection in the living tissue and proceeding bio-imaging. This choice is based on the results of our recent studies [19]. The MSGO material in the macrosize form (ceramics), synthesized in the laboratory, has showed excellent optical properties. It possesses intensive 650 nm PersL after irradiation with 263 nm light or X-rays. Preparation work for nanopowder MSGO synthesis is currently under way. Its optical properties will be later examined, and it will be prepared for analysis in living cells.

The bioapplicability of the second and third group particles will be evaluated at the Latvian Biomedical Research and Study Center (LBMC) – a long-time cooperation partner of our institute. Therefore, the proposed research has an interdisciplinary nature, combining physics, chemistry, and biology.

The research is implemented in the Laboratory of Spectroscopy. There are all the necessary conditions for successful research. The research team consists of experienced and young scientists as well as students, who can work on their bachelor´s, master's and doctoral theses. In addition, all the necessary equipment is available for spectral and structural characterization and synthesis of the new red-infrared PersL materials. Considering the analysis of the above-mentioned materials, we have chosen several new groups of materials, which could be prospective as biomedical sensors.

Future activities

For the successful realization of the project aim, we are continuing our work on the particles for biomedical applications. This includes synthesis, testing and stability evaluation of various solid-state nanomaterials. Our planned future activities are:

- Development of new low temperature synthesis methods for doped carbonate/phosphate materials (from the second group mentioned above), which are prospective for bio-application.
- Development of methods for nanomaterial creation from the prospective materials (materials from the second and the third groups).
- Versatile characterization of the structure of the obtained materials.
- Comprehensive characterization of the spectral properties of the obtained materials, based on luminescence observed under different types of excitation (UV – visible light, X-rays etc.), together with the studies of the long-lastingness of luminescence afterglow. This allows revealing of the PersL mechanisms. These studies together will allow choose the red PersL emitting material with the most appropriate properties for biomedical applications.
- Testing of the selected new materials in the Biomedical Research and Study Center.

Networking

Latvia:

- Latvia, Riga Technical University, Latvia. Dr. I. Steins. Synthesis of solid-state materials;
- Latvia, Biomedical Research and Study Center (BMC). Dr. A. Zajakina. Particle testing for applications in biomedicine;

Abroad:

- France, Universite de Bourgogne-Franche-Comte, Besancon, France. Dr. C. Ramseyer. Expertise in biomaterials;
- France, l'Institut national de recherche pour l'agriculture, l'alimentation et l'environnement (INRAE). Dr. S. Zaidi. Particle testing for applications in agriculture;
- Ukraine, National Academy of Sciences of Ukraine, Institute of Physics, Department of Physics and Biological Systems. Dr. G. Dovbeshko. Expertise in biomaterials;
- Oman, International Maritime College Oman (IMCO). Dr. M. Al-Hinai. Synthesis of nanoparticles, toxicity assessment;
- Rwanda, University of Rwanda. Dr. A. Nsabimana. Synthesis and testing of nanoparticles.

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ULTRA-WIDE BANDGAP SEMICONDUCTOR TECHNOLOGIES

State of the art.

The evolution of semiconductors in microelectronics has shown a growing preference for materials with wider bandgaps. This trend, driven by the rising demand for advanced semiconductor devices, has led to ongoing exploration of more optimal materials. Among these, Ga_2O_3 is now regarded as a promising candidate for many applications (see power electronics). Energy efficiency is at the heart of the European Union (EU) energy strategy, therefore, the creation of more efficient power electronics by increasing power density and power conversion optimization will enable significant CO_2 emission reduction. Si-based device performances degrade at high temperatures, restricting their use for high power electronics, while currently actively studied ultra-wide bandgap (UWBG) semiconductors (E_g > 4 eV), in comparison to already well-developed GaN and SiC technologies, should bring additional advantages to power devices with the ability of sustaining very high voltages, low losses for switching, high operation temperature, necessary in applications for grid, data centres and trains, electrical vehicles, aircrafts and ships.

The research objectives of the “Ultra-wide bandgap semiconductors technologies” are closely related to the ‘Key Enabling Technologies’ (KETs) - ‘Advanced Materials, Photonics, Nanotechnology and Micro- and Nanoelectronics’ identified in the European Union (EU) scientific strategies. It is fitting into the Latvian Research and Innovation Strategies for Smart Specialisation (RIS3), topics ‘Smart materials, technology and engineering’ and “Smart energy’, and the project is compliant with national Research Priority Area of ‘Technologies, materials and system engineering for increased added value products and processes, and cybersecurity’ under the Latvian Government 6th growth priority ‘Advanced knowledge base (basic science and scientific infrastructure) and human capital in areas of knowledge, in which Latvia has a comparative advantage and which are important in the process of transformation of the national economy’. It will invest new knowledge in research and innovation for the materials for next generation power electronics, enabling variety of novel products and technologies in future generations, and is in compliance with Latvia’s Semiconductor Manufacturing Memorandum of Understanding, which has been signed by the main stakeholders in Latvia, solidifying a commitment to nationally develop semiconductor manufacturing capabilities, thus increasing EU independence from other global chip manufacturers, as per the ‘Chips Act’, to “bolster Europe’s competitiveness and resilience in semiconductor technologies and applications, and help achieve both the digital and green transition”.

Our position

Thin Films Laboratory (TFL) primarily focuses on the deposition of a diverse range of inorganic materials using various deposition techniques – magnetron sputtering, including High Power Impulse Magnetron Sputtering (HiPIMS), thermal and e-beam evaporation, Pulsed Laser Deposition (PLD), Metal Organic Chemical Vapour Deposition (MOCVD), and Atomic Layer Deposition (ALD). The laboratory's current scientific projects are dedicated to the development of novel advanced materials and coatings. A list of selected publications and patents related to this activity is given below [1-9]. These activities were mainly financed by national Latvian Council of Science (LCS), European Regional Development Fund (ERDF) and Horizon Europe projects:

- A new magnetron sputtering method for the deposition of gallium oxide and its solid solution thin films has been developed.
- European Patent EP22195507.3 "A method for reactive magnetron sputter deposition of gallium oxide thin films," authors: A. Azens, M. Zubkins, E. Butanovs, J. Purans.
- Scalable epitaxial gallium oxide thin film deposition using the metal-organic chemical vapor deposition (MOCVD) method has been demonstrated.
- New insights into the physical processes of gallium oxide thin film growth and its phase stability have been acquired.
- Nine scientific articles have been published in high-impact-factor journals.
- Successfully implemented projects: ERAF No. 1.1.1.1/20/A/057 and LZP FLPP No. lzp-2020/1-0345.
- A new "Horizon Europe" RIA project No. 101172940, "Safer and More Reliable WBG/UWBG-Based MVDC Power Converters" (SAFEPOWER) (2024–2028), has been initiated.

Pulsed laser deposition (PLD) is a valuable tool for the production of thin films and epitaxial heterostructures from various materials with complicated stoichiometry. PLD allows a one-to-one transfer of elements from target to substrate, what is a strong advantage for the deposition of multiple element systems. Different atmospheres (Ar, O_2, N_2, H_2, H_2S) of deposition allow varying of properties of films in a wide range: ZnO, Ga_2O_3, MoS_2, etc.

MOCVD reactor Aixtron (AIX-200RF) is available for the synthesis of epitaxial thin films using liquid metal-organic compounds and gaseous non–metal chemical hydride and oxide gases. The equipment is suitable for the synthesis of classic LED structures, Si, ZnO, and group-III nitride 1D nanostructures, as well as for deposition of UWBG Ga_2O_3 thin films and multilayers for optoelectronic and electronic applications. There is a possibility to dope the materials, to obtain n- or p-type conductivity.

Future activities

Our ambition is to develop and to assess the first spinel – earth-abundant and non-critical oxide materials – power electronics technology platform. We will elaborate UWBG ZnGa2O4, MgGa2O4 and MgAl2O4 spinel epilayers with electronic properties required for their application in beyond the state-of-the-art high-power (> 6-10 kV) rectifiers and metal oxide semiconductor field-effect transistors (MOSFET) devices. Spinel alloying enables expansion to larger bandgaps, while engineering cation inversion provides a playground for tuning electrical properties. Understanding of the underlying physical mechanisms, as well as demonstration of Schottky diode and unipolar MOSFET device structures will pave way for further exploration into bipolar spinel technologies. The spinel platform will extend the frontier of WBG technology and address several existing issues, enhancing the devices' figure-of-merit, resulting in significant energy savings, and adding new aspects and functionalities. The demonstration of a promising spinel-based power device structures will significantly boost this research field promoting further applications of spinels in energy electronics (power- and opto-electronics). The innovation potential is oriented on novel materials and scalable environmentally friendly fabrication processes, which enables high commercial opportunities within the EU.

Moreover, our objective is to develop novel solar-blind far-UV light photodetector based on amorphous Aluminium Gallium Oxide (AlGaO) alloy semiconductor thin film deposited via scalable high-deposition-rate magnetron sputtering technique (GoFarUV). We propose to produce and investigate novel AlGaO semiconductor materials, and optimize their synthesis conditions to achieve photoelectric properties suitable for far UV light detection. Applications of such solar-blind UV-C photodetectors include environmental monitoring and space weather research, both of which are vital for addressing global climate challenges. The detectors will enable more accurate monitoring of atmospheric changes, namely ozone formation studies, and early wildfire detection, providing critical data for mitigating the impacts of climate change. Other applications include space science and technologies, security, and military.

Proposed MOCVD reconstruction is crucially important to develop the stable deposition of gallium oxide (Ga_2O_3) and $ZnGa_2O_4$ epitaxial thin films.

The main goal of activity on the Magnetron HIPIMS sputtering cluster G500M is to develop vacuum thin film deposition technologies for the stable deposition of gallium oxide (Ga_2O_3) and $ZnGa_2O_4$ thin films by reactive pulsed-DC magnetron sputtering from a liquid Ga target.

Networking

Latvia:

- Sidrabe Vacuum;
- GroGlass
- EuroLCDS; (iv)
- RD ALFA Microelectronics;
- AGL Technologies.

Abroad:

- Stockholm, Royal Institute of Technology (KTH);
- Stockholm, RISE - Research Institutes of Sweden;
- Department of Engineering Sciences, Uppsala University;
- Fondazione Bruno Kessler, Centre for Materials;
- Germany, Fraunhofer Institute or Surface Engineering and Thin Films IST Braunschweig;
- Norway, Institute for Energy Technology (IFE);
- Taiwan, National Sun Yat-Sen University.

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ANALYSIS OF PARAMAGNETIC DEFECT STRUCTURE IN FUNCTIONAL MATERIALS

State of the art

The functionality of solid-state materials is inextricably linked to structural imperfections on an atomic scale. Point defects are responsible for the mechanical, thermal, chemical, electrical, magnetic and optical properties of materials. Peculiarities of intrinsic defect formation and activator ion incorporation have been well-documented in high symmetry hosts, e.g., simple oxides and halides [1,2]– point defects can be categorized into electron centers, hole centers, interstitials and substitutional defects. The defects can occur in different charge states, often require charge compensation, may be localized at impurity ions and even form pairs and composite defect structures; therefore, their properties and stability vastly differ. As it stands characterization of point defects in lower symmetry systems with several cationic and/or anionic positions in the crystal lattice is still an ongoing quest in fundamental science. Some examples of recent results published in top-tier journals include the identification of intrinsic defects and rare earth impurities in optical materials [3–5], determination of defect structure and thermal stability in irradiated oxides, incorporation and properties of transition metal ions in biomaterials [6,7] and others.

A key aspect in the characterization of point defect structure in complex matrices is the application of advanced spectroscopic techniques. Electron paramagnetic resonance (EPR) spectroscopy has been established as the central method for the investigations of paramagnetic centers in solids allowing unambiguous identification of the defect model and its local structure. A modern approach includes variable temperature multifrequency EPR measurements, double resonance experiments, pulse techniques, and spectra simulations in correlation with complementary investigatory techniques aided by theoretical calculations.

The formation of defects in solids provides opportunities for applications of EPR spectroscopy in interdisciplinary research, industry and daily life [8–13]. In many cases, it is an unambiguous technique for quantifying paramagnetic defects in relevant materials, e.g., nitrogen centers in diamond [8]. EPR can now be used for the improvement of battery energy storage via the imaging of redox processes occurring on the actual surface of electrodes in real time while the battery performs charging and discharging cycles (in operando) [9,10]. Additionally, the accumulation of paramagnetic centers upon ionizing radiation enables the use of EPR spectroscopy in dating and provenance studies [11] as well as retrospective dose assessment [12], including potential emergency dosimetry applications [13].

Our position

ISSP UL has a continuous wave (CW) Bruker EPR system with multifrequency (X and Q band) capabilities in variable (4-300 K) temperature range with possibilities to conduct electron nuclear double resonance (ENDOR) experiments at the X band. There is also a custom-built optically detected magnetic resonance (ODMR) setup for the studies of luminescence mechanisms and the origin of optical absorption bands in materials. Advanced complementary spectroscopic techniques are also accessible at ISSP UL.

The EPR group of the Laboratory of Spectroscopy has expertise in defect analysis in systems ranging from single crystals [14–16] and polycrystalline materials [17–31] to nanomaterials and composites [32]. The main research activities are performed on inorganic solid-state materials to identify and analyze the presence of paramagnetic species – intrinsic defects and activator ions – and their role in the performance of the material. Investigations are performed on already established as well as novel phosphors, which operate in the visible [20,21], near-infrared [24,25], and ultraviolet [22,23] spectral ranges. EPR spectra simulations provide information on the oxidation state and site occupancy of luminescent ions, which is particularly insightful in complex hosts where multiple sites are available for substitution. A focal point of the group is defect analysis and engineering of smart photochromic materials [19] and persistent luminescence phosphors [20–23]. Identifying the defects responsible for the material's functions paves the way for tailored material design with optimised characteristics. Research activities are also performed on systems where the accumulation of defects yields detrimental effects [14,15,17,18]. Based on these results, guidelines for sample synthesis and recovery via thermal treatment post-irradiation can be provided. In other cases, EPR analysis of radiation-induced paramagnetic centers is used to probe the structure of the material [30,31].

Understanding the structure-property relationships enables us to advance the knowledge base relevant to fusion, optical materials and biomaterial applications. The EPR infrastructure at ISSP UL, access to complementary spectroscopic techniques and irradiation sources, as well as proficiency in materials synthesis, are attractive aspects for leading research groups in the field ensuring high-quality collaboration opportunities and research.

Future activities

- Radiation defect creation and evolution in functional materials, including materials for fusion applications. Determination of defect local structure models and their stability characterization via correlated EPR and thermal annealing experiments. A prospective collaboration with the Institute of Chemical Physics, University of Latvia is ongoing to investigate the thermal properties of radiation-induced paramagnetic defects in potential solid-state candidate materials for tritium breeding in future thermonuclear fusion reactors [17,18]. First-principle calculations have been implemented to explain the experimental EPR data of an X-ray-induced center in $LiYF_4$ single crystal [15]; it is planned to extend this approach to other single crystal materials, *e.g.*, $Gd_3Ga_5O_{12}$.

- Intrinsic defect and activator ion characterization in optical materials – luminescent and persistent phosphors, photochromic materials, optical temperature sensors. Establishing the role of defects in optical processes via combined optical and magnetic resonance techniques: EPR measurements during luminescence and ODMR. Recent results provide valuable insights into paramagnetic defect contribution to optical properties of complex materials [19–25]. A methodology for correlated EPR and luminescence (decay kinetics, thermally stimulated luminescence) measurements has been implemented within the group. The methodology will be further developed. Defect engineering of persistent phosphors is planned based on the recently published results on persistent luminescence mechanisms [20–23].

- Studies of paramagnetic defects and impurities in biomaterials. Development of variable temperature multifrequency EPR methodology including ENDOR and pulse (in collaboration with other groups) techniques. Joint investigations have expanded the knowledge base of substitution mechanisms of impurity ions and the creation of radiation-induced defects in calcium phosphate materials [26–31]. The group at ISSP UL has obtained know-how in advanced EPR methodology and spectra simulations. Insights into radiation-induced defect formation and properties have been obtained in different polymorphs of calcium pyrophosphate [30] and brushite [31], and it is planned to expand the studies on other complex calcium phosphate hosts, *e.g.*, monetite and whitlockite.

- Nanomaterials and nanocomposite materials ranging from nanoparticles, thin films to multiphase functional materials.

Networking

Latvia

- Latvia, Institute of Chemical Physics, University of Latvia, Laboratory of Radiation Chemistry of Solids; Dr. Gunta Kizane; radiation-induced defects in tritium breeding materials.
- Latvia, Light Guide Optics International.

Abroad

- Lithuania, Vilnius University, Sol-Gel Chemistry Group; Prof. Hab. Dr. Aivaras Kareiva, prof. Dr. Aleksej Zarkov; applications of advanced EPR in biomaterials.
- Poland, Institute of Low Temperature and Structure Research; Prof. Dr. Hab. Lukasz Marciniak; investigations of optical materials under high pressure.
- Poland, Institute of Low Temperature and Structure Research; Prof. Dr. Hab. Dariusz Hreniak; transparent ceramics for optical applications.
- Romania, Babes-Bolyai University. Faculty of Environmental Science and Engineering; Prof. Dr. Alida Timar-Gabor; quartz dating using EPR spectroscopy.

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SYNCHROTRON RADIATION SPECTROSCOPY OF SCINTILLATORS

State of the art

Scintillation is luminescence induced by ionizing radiation in transparent dielectric media. Nowadays, scintillator detectors play an irreplaceable role in high-energy physics (HEP), spectrometry of low energy γ-quanta, applications in medical imaging, safety systems, space applications, well and mud logging [1].

The search and development of scintillators in the last decades has been mainly focused towards higher light yield and better proportionality in order to improve the energy resolution at high energy to detect narrow states like the Higgs boson over a large background and at low energy for precise spectroscopy in applications like homeland security. Recent years have seen the emergence of fast timing capability as a new requirement, mainly driven by high-energy physics to cope with higher event rates while minimizing pile-up and time-of-flight positron emission tomography medical applications to improve the image signal-to-noise ratio [2]. Timing resolution in the 10 ps range are required in both cases, which boosts the research into scintillators with a high light yield, a short rise and decay time, as well as into ultrafast scintillation mechanisms to produce prompt photons [1-3].

Nowadays the development of scintillator materials is focused on the improvement of scintillation light yield and the increasing of time resolution. In the first domain last decade many efforts have been applied to the development of Ce^{3+} doped mixed garnets ($A_3(Ga,Al)_5O_{12}$, where A= Gd^{3+}, Lu^{3+}, Y^{3+}, Tb^{3+}, Yb^{3+} and their combinations) [4-7] and silicates (A_2SiO_5, where A=Lu^{3+}, Y^{3+} and their combination) [8-11]. In the case of mixed garnets the light yield up to 55 000 photons/MeV have been obtained [6] . The best light yield observed in silicate is a bit lower than in mixed garnet. Nevertheless, both compounds are considered to be the most prospective candidates for scintillating detectors for new CMS (Compact Muon Solenoid) developing and constructing in new calorimeter in CERN. It worth noting that currently there is no any reliable explanation of high light yield output in complex garnets and silicates. Work in this direction is currently being actively carried out by many scientific groups in Europe, the USA, China, Japan and Russia.

In the domain of medical applications (TOF-PET tomography, computer tomography) crucial parameter of scintillators is fast decay time in order to get coincidence time resolution (CTR) close to 10 ps. Targeting CTR time resolution 10 ps can be achieved in scintillators which are based on phenomena of intraband luminescence, Cerenkov radiation or core-valence luminescence (CVL). Among them only CVL has a relatively acceptable scintillation light yield (2000 photons/MeV), while others are much weaker [12]. CVL receiving renewed interest for use in fast timing radiation detection applications as a result of recent advancements in photosensor technology, readout electronics, and improved crystal synthesis and fabrication methods [13,14]. The benchmark CVL scintillator crystal is currently BaF_2; however, the drawbacks of its dominant slow decay component (~630 ns) from self-trapped exciton emission that contributes to pulse pileup in high-rate environments (e.g. HEP experiments) present a need for new CVL materials with longer wavelength emission and absence of slow emission components [12, 15-17].

In any applications scintillators as ionizing radiation detectors are naturally subject to radiation influence. Therefore, the stability of their parameters under ionizing radiation and in radiation environment is mandatory. Thus, development of fast and bright scintillators should also include the search of radiation-resistant scintillation materials which is highly relevant and important for many modern applications especially HEP, neutrons visualization [18] and space applications [19].

Our position

The development of scintillating materials is well-supported by the research infrastructure of the Laboratory of Spectroscopy. The laboratory's infrastructure has all necessary experimental capabilities for the successful research in the field of scintillating materials involving materials synthesis, structure analysis and spectroscopic characterization including time-resolved technique (tuneable picosecond laser and pulsed X-ray and electron beam setups) with picosecond time resolution. Advanced experiments based on synchrotron methods have been carried out by group members on the European synchrotron centres MAX IV (Sweden) and DESY (Germany). The FinEstBeAMS beamline at MAX IV has an end station called FINESTLUMI, while SUPERLUMI end station is installed on the P66 beamline of PETRA III storage ring at DESY. Both facilities have been intentionally designed for time-resolved spectroscopic studies of scintillating and luminescent materials. It is worth noting that some of group members played a key role in the design, construction and installation of FinEstBeAMS beamline [20, 21] and FINESTLUMI endstation [22, 23]. They are capable to examine materials of interest under picosecond synchrotron pulses in vacuum ultraviolet and soft X-ray spectral range, which perfectly fits for the successful development of electronic structure of scintillating materials, as well as for understanding the mechanism of ultrafast scintillating processes therein. The members of the Laboratory of Spectroscopy have an extended and long-term experience in synchrotron-based experiments.

It worth noting that the development of relevant CVL scintillating materials is impossible without time-resolved vacuum ultraviolet (VUV) excitation spectroscopy using synchrotron facilities. Taking into account that CVL has characteristic features like ultrafast decay time and the excitation threshold higher than 18 eV the only tuneable picoseconds synchrotron light is capable to distinguish CVL from other luminescence types. Our resent experiments at FINESTLUMI setup at MAX IV allow us to discover new type of CVL with extremely fast decay time in BaF_2-LaF_3 solid solutions [24]

Laboratory of Spectroscopy possess a vast experience in the research and development of scintillating materials. Their past work has been crucial for the study of electronic structure and luminescence (scintillating) properties of number topical scintillating materials. Recently, novel significant results have been obtained for: hygroscopic scintillating crystals SrI_2 [25], BaI_2, BaBrI [26], YAG:Ce nanocrystals [27], cryogenic scintillating material CsPbBr [28], complex oxides $SrBO_4$ [29]. Most recently, our group demonstrated pioneering results revealing energy transfer processes in one of the topical $Gd_3(Ga,Al)_5O_{12}$:Ce (or GGAG:Ce) scintillating material [30-32]. Moreover, radiation defects and damages induced in GGAG:Ce by swift heavy ions have been studied for the first time [33] and deeply analyse the obtained results with reference YAG crystals [34].

Furthermore, VUV excitation spectroscopy under synchrotron radiation is a powerful toll for the study of optical and luminescence properties of wide bandgap materials. For instance, using advantages of the photoluminescent endstation (FINESTLUMI) installed at MAX IV synchrotron facility we have recently carried out unique experiments in double activated fluoride single crystals. Excitation spectra in VUV spectral range of rare-earth ions in fluorides with meV spectral resolution have been successfully measured and deconvoluted [35-36].

Future activities

- Studies of physical mechanisms of the conversion of high-energy excitation into luminescence (scintillation) signal in topical scintillator materials: GGAG:Ce, LYSO:Ce, $CsPbX_3$ (X = I, Br or Cl), AI_2 (A = Sr, Ba) etc. The strategy to improve (modify) existing compounds to increase time resolution suitable for new generation detectors for high-energy physics and medical applications will be proposed.
- Development of red and infrared scintillators based on rare-earth doped fluorides. The main attention will be focused on the fundamental properties of rare-earth ions in vacuum ultraviolet spectral range with meV spectral resolution and the relaxation processes resulting to the infrared luminescence [17-18].
- Studies of luminescence and scintillation characteristics topical scintillator materials in form of bulk and nanocrystalline compounds in order to obtain temporal characteristics of luminescence under various excitations. The influence of synthesis parameters, as grown defects as well as reduced dimensionality on the temporal characteristics will be established.
- Investigation of radiation defects and damages as well as of the mechanism of radiation defects formation in topical scintillators to elucidate the role of defects states in energy transfer and scintillation processes.
- Expand the studies of luminescence characteristics as well as radiation defects by means of synchrotron based methods to optical materials having practical interest in nuclear physics and fusion applications. These materials ($MgAl_2O_4$, Ga_2O_3, $Gd_3Ga_5O_{12}$, Al_2O_3, MgO, Si_3N_4, etc.) do not belong to the scintillators, however the approach utilized to the study of scintillators perfectly fits for such non-luminescent materials as well [34].
- Development of ultrafast scintillator materials based on cross-luminescence phenomenon. Both theoretical and experimental engineering of fluorides to obtain cross-luminescence materials with time resolution down to 10 ps [24].
- Development of the SUPERLUMI and FINESTLUMI setups in strong collaboration of DESY and MAX IV teams in order to perform cutting-edge experiments in relevant scintillating and luminescence materials. Possible improvements of the setups should include i) design and construction of the sample holder which allow to cleave hygroscopic crystals in ultra-high vacuum in order to get fresh surfaces; ii) design and construction of the sample holder which allow to perform luminescence experiments under VUV excitations for crystals under high pressure; iii) design and construction of the luminescence registration system working in VUV range to investigate new types of CVL.

Networking

The group has long-standing active international collaborations with research groups in:

Latvia:

- Baltic Scientific Instruments
- SIA Ritec

Abroad:

- Finland: Oulu University (Prof. M. Huttula and Prof. W. Cao);
- Finland: Turku University (Prof. M. Lastusaari).
- Germany: Photon Science Division at DESY (Dr. Aleksei Kotlov);
- Sweden:MAX IV Laboratory, Lund University (Dr. K. Chernenko and Dr. K. Klementiev);
- Estonia:Tartu University (Prof. A. Lushchik and Prof. M. Brik);
- Poland:Warsaw University (Prof. A. Kaminska and Dr. Y. Zhydachevski);
- Serbia:Belgrade University (Prof. M. Dramicanin);

- Czech Republic:Institute of Physics (Prague) (K. Bartosiewicz);
- Kazakhstan:Gumilyov Eurasian National University (Dr. Z.T. Karipbaev).

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PHASE RETRIEVAL METHODS FOR ADAPTIVE OPTICS, IMAGING AND PHOTONICS

State of art

Adaptive optics remains an intensively studied field in optics. It is mainly used in astronomy to correct the effects of atmospheric turbulence on the quality of images and in vision science to correct the ocular aberrations and to improve the visibility of photoreceptors in retinal imaging. In astronomy, near diffraction-limited performance of astronomical telescopes has been achieved. In vision science, single photoreceptors, blood cells and other retinal features can be resolved. The publications mentioned below demonstrate the significance of adaptive optics in astronomy and vision science [1].

While Shack-Hartmann aberrometry remains the most popular wavefront sensing method, many new methods have emerged. Such methods are often based on coherent diffractive imaging (CDI) and the computational optics. CDI and the computational optics deals with retrieving the phase of a wave from intensity measurements. An example of the activities performed in the field of CDI is provided in papers of institutions worldwide [2]. Starting from the first algorithms retrieving the phase of a wave from intensity measurements by Gerchberg and Saxton, many new algorithms have been developed until now. These methods combine various nanostructuring methods and diffractive analysis. [3]

In order to increase the computational efficiency of phase retrieval algorithms and make these systems practically applicable, they are often embedded into computational architectures. These architectures are often based on digital signal processors (DSP), field programmable gate arrays (FPGA), graphical processing units (GPU), application specific integrated circuits (ASIC), and others. Such embedded systems make phase retrieval in real-time feasible. The use of embedded systems for phase retrieval have been reported in many research papers [4].

Phase retrieval methods can be grouped into five approaches:

- iterative methods (Gerschberg-Saxton, Fienup) [5];
- “lifting” and semidefinite programming methods (PhaseLift, PhaseMax, PhaseCut) [6];
- Non – lifting relaxation gradient descent methods (Amplitude & Wirtinger Flow) [7];
- SPARSE methods and novel approaches [8];
- Neural Networks and AI [9].

Our position

The main directions of research in Laboratory of Visual Perception involve:

- Developing and optimization of adaptive optics systems with novel wavefront sensors;
- Theoretical and practical development of optical phase retrieval methods,
- Development of prototypes using smart materials/devices with controllable optical properties;
- Development of devices and methodology for astronomy and free-space optical communications.
- Optical devices for AR/XR applications.

Based on the updated infrastructure and the acquired skills in lithography, silicon technologies, micro- and nanostructuring, the research area could be extended to include studies on micro- and nanoelectronics and photonics, MEMS systems, photonics such as light sources, photovoltaics, quantum optics, as well as use of electrically controllable materials in design of modern optical and photonic prototypes for practical applications.

The Laboratory of Visual Perception has a strong historic background fields of:

- adaptive optics in the visible and infrared region of the spectrum;
- wavefront modulator technologies;
- development of advanced micro-optical elements;
- tuneable optical elements and their use in virtual reality and vision appliances;
- optical phase retrieval algorithms; phase retrieval in a turbid and scattering optical media;
- fabrication of thin absorbing films;
- simulation of photonic structure;
- smart human-centred illumination;
- hyperspectral imaging and analysis.

Phase retrieval methods and vision related technology is currently the most actively studied fields. The laboratory has adaptive optics systems and two kinds spatial light modulators (SLM). Various thin film stacks and nanostructures are developed and investigated for needs of phase retrieval and holography. The Laboratory of Visual Perception has access to powerful simulation tools. Both metamaterials and core-shell nanostructures are first simulated and then synthesized to be included in waveguides which are further integrated into the optical setup for phase retrieval.

In cooperation with other labs, core-shell nanostructures and stacks of thin films acting like perfect absorbers have been fabricated and evaluated. These structures can be used in phase retrieval, however other applications include but are not limited to solar cells, energy harvesting, Raman spectroscopy etc.

Several projects in the field of vison, adaptive optics and diffractive imaging have been completed recently. Resulted in number of topical successful publication in period from 2017 to 2024 [10-23].

Those included postdoctoral projects, innovation projects for novel wavefront sensors, participation in the ESA programme, modeling activities under state innovation programme in photonics. The scientific activities are also facilitated with support of University of Latvia Foundation. The skill of the team resulted in participation in the LIDA voucher programme with local companies.

Recently, the Laboratory of Visual Perception has focused attention to absorbing thin films finding many applications not only in optics and photonics, but also in energy harvesting, stealth technology, light sources etc. Such materials appear to be very promising for applications in waveguides and phase retrieval and provide opportunity to develop advanced technologies in wavefront sensors. The Laboratory of Visual Perception has also started to carry out research in his field together with the partners from KTH. [19]

Future activities

Continued:

1. development of accurate and computationally effective phase retrieval algorithms for optical applications, including holography, vision research, photonics will be provided. [10-23]
2. research and development, and implementation of novel type of wavefront sensors will be activated. The new wavefront sensors foreseen for biomedicine and astronomy are based on phase retrieval approach from intensity measurements. This applies also to general optical applications, thus improving their performance and resolution of optical systems [16].
3. development of optical and smart materials and methods to expand opportunities in medical imaging. Controlled focusing through scattering media. [17].
4. study of free-space optical communication via orbital angular momentum technology [18].
5. embedding the phase retrieval algorithms into computational architectures based on digital signal processors and field-programmable gate arrays [19, 20].

The number of future specific activities are listed below:

- development of advanced microoptics for phase retrieval.
- studying the optical properties of thin films and nanostructures applicable for phase retrieval.
- development of FPGA-based systems for phase retrieval in real time.
- fabrication of absorbing thin films based on plasmonic nanoparticles/nanostructures and interference;
- nanostructures for SERS applications;
- tunable optical elements – adaptive optics deformable mirrors, tuneable lenses.
- optical system metrology on macro and micro levels.
- imaging in scattering media including tissue optics and underwater imaging.
- developments for visual optics and XR/AR applications.

Networking

Latvia:

- Optometry and Vision Science Department of UL,
- Institute of Astronomy UL,
- SIA Eventech,
- SIA HeePhotonic;
- SIA VLAVI,
- SIA ALMIKO.

Abroad:

- Sweden, KTH Electrum Laboratory; Andreas Hallen, Mattias Hammar.
- Sweden, KTH Visual Optics research group, Linda Lundstrom.
- Lithuania, Vilnius University Lighting Research Group, Prančiskus Vitta.
- Spain, Universidad de Murcia, Laboratorio de Optica (Murcia, Spain), Pablo Artal group.

- Portugal, University of Minho , Joao Linhares.
- Dublin, University College Dublin, Centre for Biomedical Engineering; Brian Vohnsen.

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ADVANCED MATERIALS FOR ENERGY

MATERIALS FOR BATTERIES

State of the art

European Long-Term Climate Strategy aims for European Union (EU) to be climate-neutral by 2050. Batteries play an important role in providing decarbonization of EU economy and enabling sustainable electrification, both for the transport sectors and grid-scale energy storage [1–2].

Current state-of-the-art batteries are largely based on lithium-ion chemistry. However, the demand for higher energy density and improved electrochemical performance in general require short- to medium-term improvements. In parallel, sustainability-related issues (i.e. material availability and toxicity) drive the development of post-Li-ion batteries [3].

Since commercialization of Lithium ion batteries (LIBs) in 1991, the gravimetric energy density of LIBs has more than doubled [4], the research and development of LIBs is ongoing. Industry currently in generation 3b of LIBs [5], with Nickel-Cobalt-Manganese oxide (NCM) ($LiNi_{1/3}Co_{1/3}Mn_{1/3}O_2$, proportion of nickel is increased from NCM 111 to NCM 811 and advancing beyond) cathode in most advanced batteries along with Si-supplemented graphite anode and liquid electrolyte. A parallel track with LFP cathodes exists. Subsequent developments are widely believed to be related to high energy NCM or high voltage spinel (HVS), all-solid-state batteries, and Li/S or Li/O_2 technologies further out in the future [4], while a parallel track of $LiFePO_4$-based materials and alternatives to LIB technology have emerged, dictated by sustainability and material availability related questions**.**

Other emerging battery types are Na-ion, Mg-ion, Ca-ion, Al-ion, metal-sulphur, anion shuttle, metal-air, semi-solid flow and redox-flow batteries. Out of these, sodium-ion battery (SIB) technology is the most mature and has a high potential for further growth, especially for application in grid-level energy storage and budget EVs. With sodium being the 6th most abundant element in Earth's crust, the raw materials are more readily available and costs – significantly lower. While the high-rate capability, stability and recyclability of SIBs are considered very attractive [8], cycle life and energy density still need to be improved [5]. This can be done by both optimizing the existing materials and developing new ones – the latter strategy along with developing fundamental understanding of the solid-state electrochemistry of Na intercalation is often considered to be the most efficient approach.

For SIBs specifically, traditional liquid electrolytes produce solid electrolyte interphases (SEIs) that are often not sufficiently stable and are likely to cause severe polarization [6]. This prompts for developments in electrolyte or artificial engineering of SEI via coatings. Another interesting approach is the use of ionic liquid (IL) -based electrolytes. In this case, a new class of materials is created when ionic liquid (IL) molecules are integrated into polymer chains. These are called polymeric ionic liquids (PILs) and provide an added benefit of mechanical and design flexibility and of the possibility to be fabricated into desired thickness and shapes, albeit at a cost of decreased ionic conductivity [7]. A mixture of PIL and sodium salts can be classified as solid polymer electrolyte (SPE) [7].

Currently most of the applied research is focused on developing new materials and improving specific power and energy densities of existing materials [8,9] as well as evaluating cycle life (service life) of battery electrodes, cells and modules [10, 11]. Developing of solid state and polymer electrolytes is another topic of interest. On a fundamental level, characterizing mass transport and related electrochemical reactions on a nanoscale is recently receiving increased attention from scientific community [12], and further improvements in materials is expected at least in part to stem from a deeper understanding of these issues.

Our position

Development of electrodes and electrolytes for Li-ion and Na-ion batteries

- LIB electrode material development focused on layered transition metal and olivine cathodes, as well advanced anodes: reduced graphene oxide, carbon nanostructures and transition metal oxides [9,13, 14];
- SIB electrode development: polyanionic compounds ($Na_2MP_2O_7$) and Na transition metal oxides $NaMO_2$ (M – Fe, Mn)) as cathodes, with a focus on assessing and improving their stability in aqueous electrolytes [15, 16]
- Cross-functional LIB and SIB electrode improvements: electrode binders (focus on sustainable aqueous electrode processing), electron-conductive additives, inert protective coatings for active electrode materials [17, 18];
- Electrolyte research focused on advanced polymer – ionic liquid composite electrolytes for SIBs and LIBs [21, 22]

Cycling stability of Li-ion battery materials and cells

- Ageing of LIB cells as a function of temperature, C-rate and other parameters, including structural and compositional changes of electrodes as a function of cycling [19, 20]

This is highly relevant problem for industry and also good grounds for subsequent more fundamentally directed research.

Future activities

The expertise of Energy Materials Laboratory focuses on battery electrode development, processing and testing, strengthened through contacts with local and European battery industry. Continued investments in human and material resources are planned. The priority research directions are:

- *Materials for Li and Na-ion materials:*
  - SIB cathodes: continuation of studies on $NaMP_2O_7$, layered oxides, layered oxides for Na-ion batteries; initiating new studies on next-generation SIB electrode materials
  - LIB electrodes: material development, sustainable and industrially feasible electrode preparation for LIBs; inert protective coatings; anodes for low-temperature performance, continued studies of 2-dimensional carbon structures; overlap and collaboration with developing materials and electrodes for supercapacitors has been planned
  - Electrodes for supercapacitors: development and characterisation of materials for supercapacitors, with a focus on sustainable carbon-based electrodes.
  - Electrolytes: ionic liquids, polymer-ionic liquid composites; nanostructured and high-surface area additives (e.g. carbon-based additives – graphene, few-layer graphite, etc.).
- *Battery cell cycle life.*

  Continued development of measurement techniques: electrochemical measurements as a function of structure/composition and their changes, possible ventures into big-data and machine-learning techniques for data processing and statistical analysis.

- *Interfaces and mass transport.*
  Solid-electrolyte interphases and interphases within electrodes as a function of composition, structure, and cycling history. Mass transport within ionic and mixed ionic/electronic conductors and across interfaces
- *Develop in-situ and in-operando characterization capability* of battery materials for assessing ageing mechanisms in LIBs and SIBs by leveraging strengths of the institute in optical microscopy, Raman spectroscopy, XRD, synchrotron X-ray, gas mass chromatography, mass-spectrometry
- *Services to industry.* Electrochemical characterization, prototype assembly (coin-cells, eventually pouch-cells C < 0.1 Ah), cycle life analysis, consulting.

Material development is a general research topic that enables us to: a) build internal collaborations with fellow research groups strong in materials synthesis and b) produce publishable results relatively quickly and address more fundamental research questions, subsequently generating more impactful fundamental results via in-depth studies of the materials developed.

To increase our scientific impact, we plan to devote part of the work to interfaces and mass transport in battery materials. This is a purely fundamental research direction that allows building deeper insights into how battery materials function.

Recently, techniques based on processing large amounts of data (machine-learning, AI, big data, etc.) have been demonstrated to be of good use in predicting cycle life and future performance of battery cells. Collaboration with Centre for Solar Energy and Hydrogen Research Baden-Wurttemberg (ZSW) could be leveraged to facilitate faster development of this research topic.

Other key points:

- **Personnel development.** Continued development of personnel is needed, increasing the proportion of PhD students and young researchers relative to undergraduate students. Gradual involvement in preparation of project proposals is encouraged starting PhD level to ensure continued funding of the personnel. Preparation of high-quality (Q1) research articles is prioritized.
- **Existing facilities.** Institute's facilities currently include basic laboratory equipment, equipment for electrode coating (mixer mill automatic coater, vacuum oven, high-precision balance), battery cell assembly (Ar-filled glovebox) as well as 90+ channels for cell characterization. There are also good synthesis capabilities (syntheses in air and inert atmosphere are possible), equipment for basic structural and compositional analysis (XRD, SEM-FIB, TEM-EDX, XPS) is available.

Networking

Latvia:

- Latvian State Institute of Wood Chemistry – Galina Dobele, Aleksandrs Volperts;
- Institute of Chemical Physics, University of Latvia – Donats Erts, Raimonds Meija;
- University of Latvia Faculty of Chemistry – Arturs Viksna;
- Riga Technical University – Prof. Andris Sutka;

Abroad:

- Germany, Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW) – Dr. Mario Marinaro, Dr. Thomas Waldmann
- Norway, Institute for Energy Research / University of Oslo – Alexey Koposov

- Norway, Norwegian University of Science and Technology – Ann Mari Svensson
- Lithuania, Vilnius University, Faculty of physics – Tomas Salkus and Linas Vilciauskas
- Estonia, University of Tartu – Alar Janes

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HYDROGEN ENERGY

State of the art

The EU's Long-Term Climate Strategy aims for climate neutrality by 2050, with renewable energy and storage as key elements. Hydrogen is crucial to this transition, projected to fulfill 24% of final energy demand and create 5.4 million jobs by 2050. The EU has further solidified hydrogen's role by supporting Hydrogen Valleys, establishing a complete hydrogen value chain. This presents a significant opportunity for Latvia and ISSP UL to lead in hydrogen research and technology. Hydrogen research is prioritized within the EU, with robust funding via the Fuel Cells and Hydrogen Joint Undertaking (FCH JU). Nearly all Member States recognize hydrogen's role in national energy and climate plans (2021-2030), focusing on transport and industry. EU legislation increasingly supports hydrogen's economic integration across all sectors. However, due to limited resources, ISSP UL must prioritize its focus within hydrogen research. [1,2]

Environmentally low-impact energy harvesting is essential for a cleaner future. Catalytic pollutant reduction, especially through electrocatalytic CO_2 conversion to hydrocarbons (e.g., methane, ethylene) and photocatalytic CO_2 reformation, can significantly reduce carbon footprints. Extensive research is underway to identify optimal materials for efficient CO_2 reformation. Recent studies reveal that doping copper with elements like iodine, bromine, and chlorine achieves a high faradaic efficiency (FE) of up to 72.6%, highlighting the need for further electrode material optimization. Research into diverse dopants and cell designs focuses on enhancing FE, electrode stability, and efficiency, with nitrogen-doped graphene (N-G) showing potential to extend electrode lifespan when combined with base electrode doping. [3-5]

Photocatalytic hydrogen production and pollution treatments—such as wastewater purification, antibacterial surfaces, and gas treatments—offer promising solutions for remote locations and passive catalytic systems. In light-induced water splitting, recent advancements show hydrogen production rates of 9.8 $\mu mol \cdot mg^{-1} h^{-1}$ with Pt-TiO_2 and 100,000 $\mu mol \cdot mg^{-1} h^{-1}$ with carbon materials. Ongoing research on binary systems, like TiO_2/nanocarbon, aims to enhance charge separation and visible light sensitivity for improved efficiency. While the EU advocates for green hydrogen, this requires significant power expansion and grid adaptation, making alternative hydrogen production methods essential. Waste management, particularly with aluminum (Al)—a strategic material generating substantial waste—is increasingly critical for sustainability. Though some Al is recycled, much remains landfilled, causing environmental pollution. [6,7]

Our position

Municipalities and companies like Rīgas Siltums, Latvenergo, and Conexus have expressed interest in using hydrogen as an energy carrier to support national decarbonization efforts. Interest in hydrogen is rising, with new players such as Fokker NextGen planning a hydrogen-based aircraft production site, and Liepaja announcing a major hydrogen production plant. Studies on hydrogen's role in transport and its potential for decarbonizing Latvia's gas networks with hydrogen-enriched biomethane have been conducted. Collaboration with energy companies aims to implement hydrogen for grid balancing and off-grid solutions, aligning with national legislation and decarbonization guidelines. [8-10]

Projects introducing hydrogen to the industrial sector have been initiated, including a modular course for industry newcomers. The course is built with options to choose and pick various aspects and applications of Hydrogen, specifically tailored to the necessity of the industry. This course was first of a kind in Baltic states and has gained traction with various local industries in Latvia. In addition to novel hydrogen generation project or catalyst investigation for low-cost hydrogen production via methane pyrolysis.

Hydrogen storage and transport in displaced mediums like aluminum, methane, and methanol are promising avenues, especially with suitable catalysts. These reactions can also generate additional heat and by-products for further utilization. Recent research has advanced understanding of reaction kinetics, pH changes, and hydrogen production from aluminum, along with studies optimizing conditions to enhance H_2 production efficiency and reduce costs. [11-15]

Nanostructured catalyst development and investigation for photocatalytic pollutant degradation and material optimization such as TiO_2/WO_3, C-TiO_2 composite, CO_2 reduction. Structure and composition of carbon materials can be engineered to be versatile for various energy applications. Few-layer graphene sheet stack powder via electrochemical pulse exfoliation of graphite; this versatile material has found various applications. [16-25]

Future activities

Currently focus is put on three directions that involve development of new materials and techniques for hydrogen production, storage/transport and use. Briefly, main focus is on the production of hydrogen using catalysts, i.e., pyrolysis and water-aluminum reaction. Future activities will drive advancements in hydrogen storage, catalysts, environmental cleanup, and education to support hydrogen technology adoption, e.g., Upcoming important direction is shifting to high temperature PEM fuel cell development due to strong push from the industry.

- Research will focus on hydrogen storage in metal hydrides, nanostructured materials, and aluminum, including testing for PtG systems under hydrogen exposure. Catalyst development will prioritize methane pyrolysis, gas reforming, and in-situ CO_2 reduction, with industry collaboration to improve hydrogen production and pollution control. Environmental projects will enhance electro- and photocatalytic methods for CO_2 reduction and pollutant degradation
- Catalyst as nanostructured TiO_2, carbon, WO_3, and others
- Thermodynamic modelling (MATLAB, SolidWorks, COMSOL) optimization of materials and use-cases.
- Theoretical and educational initiatives will expand hydrogen knowledge, with updated materials on fuel cells, storage, and electrolysis.
- Equipment for gas adsorption/desorption, for gas composition analysis the mass spectroscopy and gas chromatography are also available. Equipment available at ISSP UL essential but not exclusive to this research direction includes XRD, SEM-FIB, TEM, Raman spectroscopy, FTIR, XPS. We are expanding our abilities to measure and characterize electrochemical properties of catalyst.
- We are open to industrial collaborations in material characterization and prototype assembly; including developing materials for fuel cells (primarily hydrogen), H_2 electrolysis – two-electrode (in various setups) and membrane electrolysers, and models demonstrating electrolysis. Newly acquired micro electrode set-up will be utilized in coming months to increase the precision and investigation of catalytic activity.
- Personnel development. Continued development of personnel will be a focus for hydrogen related topics, starting from entry level students up to increasing number of PhD students as well as attraction of researchers via various grants and approaches. Preparation of high-quality (Q1) research articles is prioritized.
- Facilities – outlook. Expansion in electrochemical testing channels is needed along with climate chambers ensuring constant conditions during the measurements of electrochemical cells. Small equipment for mixing electrode slurries, calendaring and drying electrodes is needed and will be

ordered within next year. Additional *in situ/in operando* investigation cells and devices, such as Raman, FTIR, etc., are planned in coming years. Continued renovation of laboratory and office space is needed to ensure both safety of the personnel and comfortable and motivating working conditions.

Networking

Latvia

- Latvian State Institute of Wood Chemistry, G. Dobele, A. Volperts: wood-based high surface area materials (combusted carbon structures) as materials for catalytic reactions
- Riga Technical University (Ass. Prof. Laila Zemite, Prof. Andris Šutka, prof. Maris Knite, prof. Arturs Medvids, Martins Vanags and others).
- Latvian Hydrogen Association (Dainis Bošs, Aivars Starikovs, P. Lesnicenoks)
- Dinex Latvia
- NacoTechnologies
- FokkerNexGen Latvian representation

Abroad:

- Slovenia, Jožef Stefan Institute, Prof. Dr. Danjela Kuscer
- Lithuania, Vilnius University, Faculty of physics (Lithuania), Tomas Salkus' and Linas Vilciauskas' research groups: specialization in Broadband High Temperature Impedance Spectroscopy of ionic and mixed ionic-electronic conductors
- Lithuania, Šarūnas Varnagiris, Marius Urbonavicius, Darius Milcius, Laboratory of Hydrogen Technologies and Materials of Lithuanian Institute of Energy
- Lithuania, Dr. Alexandr Belosludtsev, Optical Coating Laboratory
- Iceland, University of Iceland, prof. Christiaan Richter
- Iceland, IceTec (Innovation center of Iceland) Dr. Chem Guðmundur Gunnarssonr and Rauan Meirbekova, Iceland
- USA, Prof. Gonghu Li, University of New Hampshire, USA
- Iceland, Science Institute & Faculty of Industrial Engineering, Mechanical Engineering and Computer Science, VR-III, University of Iceland, Camila Pía Canales
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- Chile, Facultad de Química y de Farmacia, Pontificia Universidad Católica de Chile, Santiago de Chile , Galo Ramírez
- Switzerland, EMPA, Gurdial Blugan.

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ORGANIC AND HYBRID PHOTOVOLTAICS

State of the art

Solar energy is one of the most popular sources of the renewable energy. While most of the commercially available solar panels consist of the silicon-based cells, a lot of research is focused on other materials. The popular topics are perovskite cells due to their high efficiency [1,2], chalcogenide cells due to the abundance of raw materials [3,4], and organic solar cells due to their variety of materials and flexibility [5-7]. With the development of so-called non-fullerene acceptors (NFAs) and the development of highly efficient electron donor polymers, the efficiency of organic photovoltaic (OPV) cells has surpassed 18%. With more advanced techniques as ternary organic solar cells (TOSCs) and tandem OPVs the efficiency has reached 20% [8].

Additional effort has been made to produce hybrid solar cells, combining the best properties of various material groups. For example, hybrid solar cells with the perovskite active layer and organic material charge transfer layer. The efficiency of such cells is well above 20% [9-11].

Our position

Laboratory of Organic Materials is a prominent place in Latvia with all necessary equipment and competence to produce and investigate organic thin-film devices. The laboratory has a long experience investigating the electrical properties of organic materials, which is essential in applications as organic solar cells and sensors. In recent years, experience in device prototyping has also been actively developed and accumulated.

Electrical properties and charge carrier transport play a vital role in organic electronics. Therefore, the laboratory pays attention to investigating the energy structure and electrical properties of organic semiconductors. Energy levels of the compounds are being studied by the photoelectron emission spectroscopy (PES) and the spectral dependence of intrinsic photoconductivity. Such measurements have been used in various local and international projects. It gives information about molecule ionisation energy (IE) and the second method gives a reasonable estimation of the energy bandgap between IE and electron affinity (EA) energy [12-14]. Charge carrier mobility of electrons and holes is determined using time-of-flight (ToF) method.

The characterization of solar cells is done using solar simulator. This allows to evaluate the efficiency and possible applicability of the cells.

Future activities

Research into new original compounds in collaboration with chemists may open possibilities to discover new materials with superior properties and to create high-efficiency devices from them.

By studying previously investigated materials and exploring their combinations, it is possible to optimise the properties of thin films made from these materials, thus opening the possibility to create devices with higher efficiency.

Future directions:

- *Development of ternary organic solar cells*

We are working on the Latvian Council of Science project No. LZP-2022/1-0494 "Development of ternary organic solar cells by employing original indacene-tetraone based non-fullerene acceptors". The objective of this research project is the development of novel non-fullerene electron acceptors with one-dimensional charge transfer properties that will allow the construction of highly efficient ternary OSCs. In this project, novel non-fullerene acceptors for organic solar cells are being synthesized and investigated. Adding them to already used commercial donor and acceptor materials (electron donor polymers PM6 and PM7, as well as NFAs like Y6 and Y7) ternary organic solar cells are developed. For now we have made TOSCs with the efficiency of over 12% [15], with the quite promising short-circuit current density (Jsc) of over 20 mA/cm^2. Adding the third material in the active layer of OPV has helped to increase the efficiency of solar cells by slightly improving Jsc and fill factor (FF). For now, the FF values of around 0.60 do not allow reaching higher efficiency, yet the work on the optimization of the morphology of the cell's active layer is still ongoing.

- *Development of hybrid chalcogenide/ organic tandem solar cells*

Combining the results in this project and the results from the concluded EEA and Norway grant "Development of Semi-Transparent Bifacial Thin Film Solar Cells for Innovative Applications", while expanding the collaboration with the Tallinn University of Technology, further activities are planned. Namely, a post-doctoral project related to the development of chalcogenide/ organic tandem solar cells has been submitted. The chalcogenide (Sb_2S_3) layer would work as a top cell, collecting a part of visible light, while organic solar cell would work mostly in the near-infrared part of the spectrum. This would reduce the intensity of light reaching the bottom (organic material) cell, which should reduce the photodegradation of the organic materials and in return improve the lifetime of the cell.

Prototypes of investigated systems will be made to confirm the commercial potential of the devices.

Networking

Latvia:

- Latvia, Riga Technical University, Institute of Applied Chemistry, Prof. Valdis Kokars, Assoc. Prof. Kaspars Traskovskis

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NOVEL THERMOELECTRIC MATERIALS

State of the art

Addressing the energy crisis requires the use of renewable resources and the development of more innovative and efficient devices. Wasted heat represents a significant, yet underutilized, energy source. It is estimated that around 20% of the 15 terawatts needed annually for global power consumption is lost as low-level heat (<200°C). Thermoelectric generators (TEGs) can harness this wasted energy by converting heat directly into electricity. Effective TEGs can solve multiple problems: they use wasted heat for electricity generation, thereby reducing global warming and tackling the energy crisis. This realization has led to extensive research into thermoelectric materials, including organic materials [1–4]. At low temperatures, organic materials can demonstrate properties that are comparable to or even superior to those of traditionally used inorganic materials [1,5]. Recently, the synthesis of thermoelectric nanoparticles with a high figure of merit (ZT >1) has been reported [6,7]. Integrating these nanoparticles into suitable polymer matrices can produce valuable hybrid thermoelectric materials, such as those used in Photovoltaic-Thermoelectric hybrid systems [8,9]. The hybrid materials concept, where inorganic TEs are coupled with polymers, has gained much attention, enabling harvesting low-grade heat otherwise lost, even with a lower ZT than the inorganic counterpart. Flexible organic–inorganic hybrids are promising thermoelectric materials to recycle waste heat in versatile formats [10–12].

Our position

The Laboratory of Organic Materials in Latvia is a leading facility equipped with all the necessary tools and expertise to produce and study organic thin-film devices. With extensive experience in examining the electrical properties of organic materials, the laboratory plays a crucial role in applications like thermoelectricity, organic solar cells, and sensors. Recently, the lab has also significantly advanced its capabilities in device prototyping.

Understanding the electrical properties and charge carrier transport is crucial for organic electronics, making their study vital. Therefore, the laboratory is dedicated to investigating the energy structure and electrical characteristics of organic semiconductors. The energy levels of these materials are examined using photoelectron emission spectroscopy (PES) and the spectral dependence of intrinsic photoconductivity. These techniques, applied in various local and international projects, provide valuable insights into the ionization energy (IE) of molecules. Moreover, the latter method offers a reliable estimation of the energy bandgap between IE and electron affinity (EA) energy [13–15].

In the Laboratory of Organic Materials, full spectra of thermoelectric properties can be investigated, including Seebeck coefficient measurements in a lab-made Seebeck measurement unit, thermal conductivity measurements by 3ω technique and electrical conductivity measurements by four-probe method [16,17]. In the future, the measurements of thermal conductivity in thin films will be improved, achieving the possibility to determine the thermal conductivity in different directions in a thin layer [18].

The hybrid materials concept, where inorganic TEs are coupled with polymers, has gained much attention, enabling harvesting low-grade heat otherwise lost, even with a lower ZT than the inorganic counterpart. Flexible organic–inorganic hybrids are promising thermoelectric materials to recycle waste heat in versatile formats [10–12,19–21]. Besides, the thermoelectric effect can be used to create light sensors. [22] For example, thermopile detectors have long been known. Prototypes of thermoelectric radiation sensors with superior characteristics are created using thin films of organic materials with unique properties, achieving broad spectral range as thermopiles and high-speed performance as a photodiode. ISSP UL has patented technology as WO/20202/095126 and EP3811043 "A High-Bandwidth Thermoelectric Thin-Film UV, Visible Light and Infrared Radiation Sensor and Manufacturing Method Thereof", which have been sold to the multinational company Thorlabs. Licensing and technology transfer contract with Thorlabs GmbH was signed on 11.10.2021.

At the Laboratory of Organic Materials, research is conducted on the thermoelectric properties of glass-forming low molecular weight compounds, which are promising candidates for new hybrid thermoelectric materials. Recently, the laboratory secured a project from the Latvian Council of Science titled "Advancing Sustainable Thermoelectric Hybrid Systems Utilizing Glass-Forming Low Molecular Weight Compounds."

Meanwhile, the EXAFS Spectroscopy Laboratory has initiated a project titled "The Entropy-Driven Approach to Enhance the Thermoelectric Performance of Chalcogenide-Based Compounds," which focuses on utilizing novel thermoelectric nanomaterials.

Future activities

Further development of the energy harvesting device field will be divided into two parts. One will be performed in close collaboration with chemists from other academic institutions. The second is related to the investigation of the energy conversion system concerning morphology.

Research into new original compounds in collaboration with chemists may open possibilities to discover new materials with superior properties and to create high-efficiency devices from them.

By studying previously investigated materials and exploring the effect of morphology on energy conversion, it is possible to optimise the properties of thin films made from these materials, thus opening the possibility to create devices with higher efficiency.

Future directions:

Development of organic-inorganic hybrid system thin films for thermoelectricity

One of the primary steps in developing hybrid systems, such as organic-inorganic thin films for thermoelectricity, is the high-quality incorporation of inorganic nanoparticles into organic materials. Achieving a homogeneous distribution of nanoparticles in the thin film is crucial for the successful advancement of these hybrid systems. Understanding charge carrier transport and energy levels in solids is essential. This is particularly important in hybrid systems, where charge carrier transport can be hindered by trap levels resulting from structural defects and energy level mismatches between system components.

Organic materials typically have low thermal and electrical conductivity. Over the past decade, hybrid organic-inorganic materials have emerged as promising thermoelectric candidates, combining the low thermal conductivity and high Seebeck coefficient of organics with the high electrical conductivity of inorganics. However, these hybrids often suffer from poor thermoelectric properties due to aggregated nanostructures.

To improve this, high-quality incorporation of inorganic nanoparticles is crucial. Adding thermoelectric active inorganic nanoparticles or low-dimensional carbon structures, like carbon nanotubes or graphene, can enhance electrical conductivity and Seebeck coefficient while reducing thermal conductivity, following the “phonon-glass, electron-crystal” principle for higher ZT values.

In collaboration with Prof. M. Toprak’s group at KTH, we are researching chalcogenide TE nanoparticles to form hybrid structures and develop TE devices. We also plan to include copper and silver chalcogenide nanoparticles and other thermoelectric nanoparticles, efficiently synthesized using microwave-assisted methods from Prof. Toprak’s group.

Development of Thermoelectric generators on a flexible substrate

Organic material-based thin film deposition on flexible substrates by making flexible devices is one of the most significant advantages of organic materials. Nevertheless, several issues should be addressed before depositing a multilayer system on the flexible substrate.

1. Structuring of electrodes should be done mainly by the lithography method;
2. Thermal deposition of compounds should be done at low temperatures;
3. The thermal properties of the flexible substrate should be considered during thermal treatment of the layers;
4. Investigation of bending radius and cycles should be performed.

Prototypes of investigated systems will be made to confirm the commercial potential of the devices.

Networking

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MICROFLUIDIC DEVICES

State of art

OOC systems are microfluidic devices designed to replicate human organ functions by culturing epithelial and endothelial cells in separate microfluidic channels divided by a porous membrane. These systems allow controlled, dynamic microenvironments where cultured cells exhibit biomarker expression and activity levels similar to in vivo conditions due to applied shear and mechanical forces [1]. OOCs replicate physiologically relevant environments for cell growth and hold the potential to replace animal testing by providing more accurate, human-relevant organ-function models [2,3]. This is underscored by the FDA Modernization Acts 2.0 and 3.0, which enable the use of OOC devices alongside animal trial data in clinical trial submissions, highlighting their potential as a test bed for pharmaceutical developers and research institutions.

Our group focuses on developing OOCs with novel materials and fabrication methods, addressing the limitations of current PDMS-based devices. PDMS, while widely used, absorbs small molecules, is difficult to scale for mass manufacturing, and limits the creation of anaerobic conditions required for specific applications, such as gut microbiota modeling [13,14]. Current OOC devices mimic human organ functions by culturing relevant cell types, such as gut epithelial and endothelial cells, in horizontal microfluidic channels separated by porous membranes. These channels allow culture media flow, supplying nutrients and removing waste, enabling the formation of a confluent monolayer of cells that simulates organ tissue response to external stimuli [4]. This technology has demonstrated promise in pharmacokinetics (PK), drug toxicity, viral disease studies, and cancer research [1,4-7].

OOC systems also enable personalized medicine by incorporating patient-derived biological material, such as primary tissues, blood samples, or induced pluripotent stem cells (iPSCs), and by tuning physical and chemical parameters to mimic individual physiology [7]. This facilitates person-specific drug efficacy and safety testing, paving the way for truly personalized medicine. Current state-of-the-art applications include accurate single-organ models with representative cellular composition and personalized PK/PD studies, but the systemic response of human physiology necessitates the development of multi-organ chips [8].

Particularly, blood flow studies have greatly benefited from microfluidic technologies, which enable high-resolution modelling of vascular environments under well-controlled conditions. These systems replicate physiological and pathological flow rates, hematocrit, and vessel geometries—such as networks, bifurcations and confinement—allowing real-time observation of red blood cell (RBC) deformation, aggregation, and interactions with other cells, pathogens, or materials and the study of its detailed dynamics and rheological properties [32,33]. When coupled with advanced tools like confocal microscopy, and optical tweezers, they offer precise, quantitative insight into the cellular and molecular mechanisms underlying healthy cases and diseases like thrombosis, and hemorheological disorders [34-36]. When combined with electrical sensors, these platforms provide powerful capabilities for point-of-care diagnostics and continuous physiological monitoring [37,38].

Multi-OOC devices interconnect systems such as intestine, liver, and kidney chips to predict PK responses, utilizing either fluidic interconnects or pipetting robots for integration [1,9,10]. For example, multi-OOC systems have been used for cancer modeling and subsequent PK-PD analysis in interconnected four-organ setups [11]. However, despite numerous seminal studies, the core design of OOC chips has seen little innovation over the last decade [4,6,12].

PDMS remains the dominant material for OOC fabrication, yet its limitations hinder adoption in pharmaceutical research. The absorption of small molecules and inability to mass manufacture at scale result in high costs, while gas permeability issues prevent the creation of anaerobic conditions [13,14]. Alternative materials offer potential solutions, including cost reduction, scalability, and improved environmental control. Recent efforts from groups such as Kang [16], Jeon [17], and George (unpublished, UC Davis) have focused on non-PDMS OOCs, but no major publications have demonstrated their integration into drug development studies. Startups like Dynamic42 and BeOnChip reflect the complexity of developing PDMS-free devices, leveraging expertise from microfluidic manufacturing hubs like Microfluidic ChipShop and TE Connectivity [16,17].

Recent conferences, including the MPS World Summit 2024 and EurOOCs 2024, highlighted advances in OOC technology. ISSP UL members attended these events, which focused on sensor development for monitoring cellular metabolism and enhancing in vitro models. Particular emphasis was placed on glucose and lactate sensors, as well as oxygen sensing for gut-on-chip models to better understand gas environments in epithelial channels [25,26]. These developments demonstrate growing interest in improving OOC capabilities for specific applications.

Our position

The Laboratory of Micro- and nanodevices focuses on designing and developing novel OOC devices suitable for large-scale manufacturing. Proof-of-principle (POP) devices integrating TEER [18] and gas and pH sensors [19] have been demonstrated. By mid-2024, multiple publications on PDMS-free OOC devices made from OSTE-COC and COC materials have been published [27, 28, 29]. A recent *Biomaterials Today* (IF>8) publication shows that, using OSTE-COC materials and our manufacturing methods, patient-derived pancreatic cancer models can be sustained for over 50 days [27].

In 2022, previously developed chips supported full human microbiota culturing in gut-on-chip devices. Microbiome diversity analysis via advanced sequencing revealed that >95% of bacteria in the chip after 72 hours were strict anaerobes or anaerobes, confirming superior gut microenvironment recapitulation. Experiments also showed bacterial extracellular vesicle (EV) transfer across the gut-blood barrier. Multi-OOC experiments began in 2023, including a two-year kidney-liver-pancreas system project. The 2022 patent application was turned into a PCT application for priority retention, and the EP patent was sold to Latvian spin-off Cellbox Labs. Cellbox Labs has been using ISSP UL cleanrooms to develop chip technology and build lung-on-chip devices from injection-molded COC chips to replicate microgravity conditions on Earth [28].

In 2025, two projects will focus on TEER sensors correlating TEER values with tight junction protein expression in gut-on-chip models and a novel biomaterial test bed recapitulating a rodent calvarial critical-size defect model in an OOC platform.

Regarding oncology-related biomarkers, our core interest lies in EVs, heterogeneous vesicles released by cells like MSCs. EVs transfer molecules influencing recipient cell behavior and play roles in cancer progression and treatment [18]. They carry genetic material, proteins, lipids, and signaling molecules, mediating intercellular communication in human fluids and regulating physiological and pathological processes. EVs have emerged as potential therapeutic tools and biomarkers in cancer [21]. However, challenges remain, such as methodologies for isolating EVs from high-volume samples for clinical use [22, 23]. Current approaches include EV capture from concentrated liquids like blood plasma and analysis using lab-grade equipment.

A collaboration with Latvian Biomedical Centre (BMC) aims to develop a device for EV isolation from cell culture media and urine, improving reproducibility and reducing preparation time. The device, based on field-flow fractionation (FFF), eliminates user concentration steps. The project resulted in three publications: characterizing bifurcated asymmetric FFF systems [30], applying this method for clinical sample purification [30], and demonstrating the method in the *Journal of Visualized Experiments* [31].

New research staff are contributing expertise in blood-related microfluidics, expanding the laboratory's scope and integrating hemodynamics and blood diagnostics into our broader organ-on-a-chip (OOC) strategy. This includes the study of blood rheology, red blood cell (RBC) behavior, and cell–microbe nano and microrobots interactions under physiological and pathological flow conditions. Efforts also address the development of diagnostic tools based on flow-induced cellular responses and sensor integration. Additionally, space health is an area of growing interest, with plans to investigate hematological alterations in microgravity environments. Together, these activities reinforce our shift toward PDMS-free, scalable microfluidic systems equipped with integrated sensing technologies for clinical and translational use.

Future activities

Further work will focus on multiple models supporting necessary design changes. Our research will include sensor integration (TEER, O_2, CO_2, pH) and membrane engineering to support 3D cell arrangements, such as intestinal villi structures. We will also work on flow through modular glucose and ATP sensors for OoC models.

Future research will focus on applied microfluidics and microfabrication, emphasizing industrial or applied science applications with commercialization opportunities. OOC technology, biomarkers for oncology, and personalized medicine diagnostics remain central to our work. We prioritize scalable, large-volume manufacturing materials and integrated sensing technologies for OOC devices, aligned with biological model advancements at BMC. This includes engineering multi-organ devices and fabricating multi-organ systems on a single chip, representing human physiology for pharmaceutical applications. With an estimated EUR 4.5 billion TAM in drug discovery, OOC technology offers significant IP generation and commercialization potential.

Our biomarker research focuses on EV technology for cancer diagnostics and treatment. Short-term efforts aim to improve EV separation, while long-term goals include lab-on-chip solutions for EV capture and analysis. Current projects involve on-chip EV capturing and optical sensing, with proposals submitted with BMC and the Laboratory of Organic Materials. Collaborations include Dr. Qin Wang (RISE) on graphene sensor development, with plans to hire experienced personnel for advanced sensor integration.

We see significant opportunities in collaborating with pharmaceutical companies, as they typically rely on academic and industrial partnerships for OOC R&D. Most current OOC systems are early stage, focusing on proof of concept, with limited usability for industrial applications. Our engineered systems will integrate microfluidic devices, instruments, and optimized cell culture protocols in cooperation with BMC.

Pharmaceutical companies engaged include AstraZeneca, GlaxoSmithKline, Roche, Pfizer, Bayer, ThermoFisher, Merck, Novartis, Janssen J&J, AbbVie, Evotec, Charles River Laboratories, Covance/Labcorp, Eurofins, and Agilent.

Pharma's adoption of OOC systems is recent, offering a unique opportunity for collaboration. OOC technology can initially contribute to drug efficacy and toxicity studies, but widespread replacement of animal trials will require legislative changes and more evidence, likely over 5+ years. Strategic use of OOC technology could save 10–24% of R&D costs [24].

Future work will focus on applied microfluidics for blood-related applications. We aim to develop robust, PDMS-free microfluidic platforms suitable for scalable production and compatible with physiological fluids such as plasma and whole blood. Our immediate goal is to optimize these devices for the quantitative analysis of blood-related diseases. Integration of real-time sensors will enable monitoring of endothelial integrity and cellular metabolism in blood flow models. We will also investigate the behavior of bacterial and colloidal populations in flow, particularly their interactions with RBCs at rest and under shear, to support bacteriotherapy design, infection dynamics modeling, and to advance the field of active matter within the emerging framework of mechanical statistics. This work is carried out in collaboration with leading research groups, including the Biofluids and Biorheology Lab at the University of Ottawa (Canada), the Active and Programmable Matter Lab at ESPCI Paris (France), and the Institute of Advanced Simulation (IAS & IAS-2) at Forschungszentrum Jülich (Germany).

In parallel, diagnostic platforms will be further developed: the Thrombocheck system for point-of-care testing of thrombus formation under defined wall shear rates and geometries in collaboration with the Biofluids and Medical Device Research Group at Georgia Institute of Technology (USA), and Sicklecheck for low-cost sickle cell anemia detection from finger-prick samples using image-based or sensor-based diagnostics—aligned with tech-for-good initiatives targeting underserved regions such as Africa and India. Additionally, we aim to adapt these systems for microgravity environments through integrated sensors with telecommunications capabilities and long-term data storage. This includes the study of RBC aggregation, flow dynamics, and membrane properties under spaceflight conditions, contributing to the understanding of space anemia and other hematological alterations observed in astronauts in collaboration with the Red Blood Cell Dynamics Group at Saarland University (Germany) and the Space and Planetary Exploration Laboratory at the University of Chile to support Earth-to-orbit translational strategies with NASA. A potential collaboration with Cellbox Labs is envisioned, building on their expertise with gut-on-chip systems tested in microgravity chambers.

Networking

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- Latvia, , Latvian Institute of Organic Synthesis, K. Jaudzems group
- Latvia, Riga Stradins University, Cakstina's group

These collaborations enhance our access to diverse expertise in hemodynamics, synthetic biology, instrumentation, and international science funding.

Abroad

- Belgium, Flemish institute for technological research VITO, I. Nelissen group
- Belgium, KU Leuven, VITA group in Rega Institute
- Sweden, KTH Royal Institute of Technology in Stockholm (Sweden), A.Herland group;
- Sweden, Karolinska Institute, O. Parlak group;
- Germany, The Max Delbrück Centre for Molecular Medicine in the Helmholtz Association, Sanders lab;
- Netherlands, University of Twente, BIOS Lab on a chip;
- USA, University of Vermont, UVM Cancer Center
- USA, Iowa State University, The Anand Group;
- Canada, University of Ottawa, Fenech's Lab: Biofluids and Biorheology;
- USA, Georgia Institute of Technology, Ku's Lab: Biofluids and Medical Device Research Group;
- France, ESPCI Paris, Olivier Dauchot's lab on active and programmable matter;
- Germany, Saarland University, Lars Kaestner's Group on Red blood cells dynamics;
- Germany, Jülich Forschungszentrum, Institute of Advance Simulation IAS & IAS-2;
- Chile, University of Chile, Space and Planetary Exploration Laboratory;

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CENTRES TARGETING EXCELLENCE

OPEN-ACCESS RESEARCH INFRASTRUCTURE

To support fundamental and application-oriented studies, **OPEN ACCESS RESEARCH CENTRES** are developed and further modernized.

Fundamental research:

- ***Computing Centre:*** Hosting the Latvian SuperCluster (LASC) with advanced computing capabilities. LASC is a heterogeneous high-performance computing cluster based on reliable multiprocessor servers and running the Linux operating system, with a theoretical peak performance of about 150 TFlops. It will be upgraded in the coming years to offer significantly enhanced performance and, for the first time, provide access to high-performance graphical processors, which are essential for efficient parallel data processing in emerging technologies such as artificial intelligence and machine learning.

- ***X-Ray absorption knowledge excellence Centre*** focuses on the study of materials structure using synchrotron radiation X-ray absorption spectroscopy. It uses advanced theoretical calculations and simulations of experimental data to gain insight in the structure-property relationships in materials.

- ***Spectroscopy Centre*** conducts material science research using optical, magnetic, and electron spectroscopy. State of the art commercial instruments like FTIR Vertex 80v, Raman spectrometer TriVista CRS, Spectroscopic ellipsometer RC2-XI, photoluminescence spectrometer FLS1000, TL-OSL reader Lexsyg research, EPR spectrometer Elexsys-II E500 CW, XPS/UPS system are located in close vicinity. Custom built setups based on tunable nanosecond, picosecond and femtosecond lasers for excitation and various detection systems including Time-Correlated Single Photon Counting are available at Centre.

- ***Microscopy and Structure Analysis Centre:*** Provides cutting edge tools for macro-to-nano scale explorations: SEM Tescan Lyra 3 dual beam system; TEM FEI Tecnai G2 F20; SEM Helios 5UX (Thermo Fisher Scientific); AFM Veeco AFM CP-II; Profiler Dektak 150; Vero interferometric AFM (Oxford Instruments).

Applied research:

- ***Electrochemistry Centre:*** Research in materials for lithium and sodium-ion batteries, hydrogen technology, and electrochemical characterization: 90+ electrochemical test channels, incl VMP3 potentiostat/galvanostat (BioLogic); Ar-filled glovebox; Particle size analyses equipment Litesizer 500; Differential scanning calorimeter (DSC).

- ***Thin Films Centre:*** advanced thin film deposition services: Roll-to-Roll PVD semi-industrial large scale PVD Magnetron deposition; Epitaxial Dual Magnetron Sputtering (HIPIMS, DC, RF); Multifunctional cluster tool R&D SAF 25/50 (HIPIMS, e-beam, organic-inorganic evaporation); PLD oxide and sulphide epitaxial grows; ALD Savannah; MOCVD; AP-CVD; Spin coater Laurell WS400/WS650.

- ***Nanotechnology Centre:*** Operating a 650 m^2 cleanroom with cleanliness level ranging from ISO 4 to ISO 8 standards for micro and nanofabrication: Mask aligner Suss MAG Gen 4; EBL Raith eLine Plus; Laser writer Heidelberg MPG 101; Wire bonder F&S Bonder 53107&5332; Dry etching facility PlasmaPro 100 ICP 300; Microfluidics Pilot Line including injection moulding and ultrasonic welding tools.

THEORETICAL MATERIAL SCIENCE AND MODELLING

State of the art

Large-scale computer simulations serve as an efficient tool for designing of new functional materials, interpretation of experiments and understanding of their electronic, structural, chemical, optical and dielectric properties [1-4]. Of special importance are nowadays nanomaterials and low-dimensional systems, as well as to modelling of processes under realistic working conditions, i.e. high and low temperatures and gas pressures, harsh radiation environment, etc. Thermodynamic approach based on the first principles total energy calculations of advanced materials and their vibrational properties is very efficient [1,2]. Most of the theoretical researches are performed in close collaboration with experiments. Of great importance is understanding the specific role of impurities in materials performance, e.g. band engineering of band gaps for water splitting, photovoltaics, and in materials radiation resistance [3,4].

Our position

The two Theoretical Laboratories at ISSP UL (Laboratory of Computer Modelling of Electronic Structure of Solids and Laboratory of Kinetics in Self-Organizing Systems) focus on multiscale computer modeling of advanced materials, combining ab initio, kinetic Monte Carlo, and Molecular Dynamics methods. Our theoretical activities [5-35] cover the entire spectrum of problems mentioned above in state of the art part.

Of special importance is the design of new materials for energy applications: piezoelectrics for energy harvesting [5], fuel cells for converting chemical energy into electricity, hydrogen production through photostimulated water splitting [6, 7], optical and dielectric materials for fusion reactors [8,9], and photovoltaics [10]. This work emphasizes the impact of defects and impurities in materials relevant for energy applications.

Both labs have a strong background in large-scale first-principles computer simulations on advanced materials, their surfaces, interfaces and nanostructures. Massive parallel computer modelling combines commercial quantum mechanical codes with custom-built thermodynamic analysis, empirical potential approaches, molecular dynamics and kinetic Monte Carlo techniques. This comprehensive approach provides reliable atomic and electronic structures of complex advanced materials and nanomaterials, and a multi-scale understanding of physical-chemical processes in a variety of materials with technological applications. For instance, we study the influence of the shape and size of perovskite nanoparticles on the piezoelectricity and photostimulated water splitting based on ab initio calculations. Different ferroelectric and semiconductor particles with defined sizes and shapes of plates, cubes and/or wires are synthesized by our partners and systematically self-assembled on a substrate, e.g., for the energy-harvesting devices. We developed theory of such self-assembling process and suggest how to control this process.

Our main focus is on the following topics:

- Defects in solid state. Computer modelling of the atomic, electronic, and magnetic structure of pristine and defective solids and interfaces, including nanostructured materials [5-35].
- Materials for nuclear fusion applications [8, 9, 16, 17, 25].
- Surfaces and interfaces of materials. Calculations of surface property of nanostructured materials for efficient water splitting (e.g. 2D layered materials, titania, ABO3-type perovskites) [6, 18, 20].

- Vibrational properties of defects in materials. First principles calculations of the vibrational properties of nanostructured materials. Calculations of the IR and RAMAN spectra for hybrid nanostructures [15, 16, 17, 19, 23, 26].

- The electronic structure and processes at nanoscale. First principles calculations of electronic properties of nanomaterials and heterostructures at nanoscale [6, 18, 20, 23]. Excited state calculations of hybrid nanostructures for photocatalysis [24].

- Calculations of the properties of hybrid metallic-carbon nanotubes and semiconductor nanowires. First principles calculations of charge transfer processes in nanostructured photoelectrodes. Computer simulations of adsorption properties of Cu-decorated graphene in the presence of external electric field [29]. Analysis of mechanical properties of nanowires [30].

- Study of perspective materials to be used in UV photon sensors [6, 8, 12], water splitting [6, 7, 18, 20-24, 31], p-type conductors [12], optics for fusion reactors diagnostics and plasma heating [16, 17, 25], photostimulated hydrogen production upon perovskite nanoparticles [7, 18, 26], advanced phosphors for LED-type light sources [26, 32].

- Ab initio molecular dynamics and machine learning methods for description the structural and vibrational properties of solids and interpretation of EXAFS measurements [27, 28].

- Analysis and critical review of modelling methods and pathway search for accurate comparison of theoretical and experimental data [13, 30-35].

Future activities

Labs future activities will be focused on understanding of chemical and physical material properties in the photocatalytic processes and design of new effective photocatalysts for water splitting with hydrogen production based on perovskites crystallites and nanoparticles. This will require a combination of the band gap engineering and selection of proper catalysts, in a close collaboration with leading experimental teams in Europe Our activities in these areas are already well-recognized internationally. In most projects, we have industrial partners, which are supposed to realize our theoretical predictions into real applications.

Most of our future activities will address energy challenges, including advancements in batteries, fuel cells, photovoltaic, nuclear fuels, functional materials for fusion reactors, water splitting. For efficient water splitting using nanocrystals, we aim to identify ways to improve the efficiency of renewable energy conversion devices, focusing first on water splitting in electrochemical cells based on nano-scaled oxides.

The primary objective will be to develop multiscale modeling approaches and roadmaps that integrate various state-of-the-art theoretical methods, enabling comprehensive and advanced predictions of material properties. This effort aims to bridge knowledge gaps between different theoretical methodologies and computational codes, facilitating the discovery of novel materials for energy conversion. We will conduct large-scale computer simulations of various nano-materials, particularly those based on ABO3 perovskites and complex oxides, modeling water splitting processes, intermediate products, and assessing efficiency based on polarity and composition. In collaboration with top European experimental teams, we will also integrate machine-learning approaches with advanced computational techniques, including non-adiabatic molecular dynamics (NAMD) and time-dependent DFT (TDDFT), to understand and predict properties of heterojunction photocatalysts and defect-induced properties of solids.

Another key objective is the theoretical prediction of new cathode materials for fuel cells that can effectively operate at intermediate temperatures, transforming chemical energy into electricity. This requires understanding of: (i) the decisive structural properties for sufficient proton conductivity; (ii) conditions for the majority of proton uptake by acid-base water incorporation or by redox reaction; (iii) link between mechanical properties and water incorporation. The primary target materials of the proposed research are perovskite-type ferrites and cobaltites.

Key research directions and objectives for developing materials in sustainable energy applications:

- Development of multiscale modeling approaches and roadmaps for advanced materials modelling.
- Use of machine learning for design of new nanomaterials as well as optimization of heterojunction photocatalysts and other electrochemical reactions.
- The improvement of water splitting on faceted surfaces of perovskite nanoparticles and doped semiconductors.
- Oxygen and hydrogen production mechanism, kinetics and thermodynamics upon water splitting.
- The role of defects and dopants in epitaxial growth of thin films.
- Calculations of the excited states of insulating and semiconducting materials.
- The properties of defects in the bulk, thin films and surfaces of binary and complex halides and oxides.
- Advanced new materials for photovoltaics, halide perovskites, LED light sources.
- Modelling and improvement of proton ceramic fuel cells based e.g. on double perovskites.
- Employing DFT and molecular dynamics to interpret and validate experimental data on various materials, including nano- and heterostructures.

Networking

Abroad:

- Belgium: Namur Institute of Structured Matter, University of Namur, Dr. M. Achehboune
- China: Chongqing University of Posts and Telecommunications, Prof. C-G. Ma
- Estonia: University of Tartu, Prof. A. Lushchik. Prof. M. Brik
- Germany: DESY, Hamburg, Dr. A. Kotlov; Karlsruhe Institute of Technology (KIT), Prof. T. Scherer; Stuttgart, Max Planck Institut für Festkörperforschung, Dr R. Merkle; University Duisburg-Essen, Essen, Prof. K. Exner; MBN Research Center gGmbH, Prof. A.V. Solov'yov;
- Greece: Aristotle University of Thessaloniki, Prof. J. Kioseoglou
- Italy: University of Turin, Prof. R. Dovesi
- Israel: Technion, Prof. M. Toroker; Weizmann Institute of Science, Prof. I. Lubomisrsky
- Japan: Waseda University, Tokyo, Prof. T. Yamamoto
- Kazakhstan: L.N. Gumilyov Eurasian National University, Astana, Prof. Dauletbekova; Institute of Nuclear Physics, Astana, Dr. M. Zdorovets
- Poland: Jan Długosz University, Częstochowa, Prof. M. Piasecki
- Serbia: Vinča Institute of Nuclear Sciences, University of Belgrade, Prof. M. Dramićanin
- Slovenia: Ljubljana, Jožef Stefan Institute, prof. M. Kržmanc
- Spain: Madrid, CIEMAT, Dr. R. Vila
- Switzerland: Paul Scherrer Institute, Dr. M. Krack
- Taiwan: Taiwan National University, Prof. J.C.S. Wu
- Ukraine: Berdyansk State Pedagogical University, Zaporizhzhia, Prof. Yana Suchikova; Lviv Polytechnic National University, Prof. H. Klym
- USA, University of Maryland, Dept of Materials Science and Engineering, Prof. M. Kuklja

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SPECTROSCOPY TECHNIQUES FOR ADVANCED MATERIALS RESEARCH

State of the art

With the advancement of modern science, the investigation of materials at the atomic and molecular scales has increasingly relied on sophisticated spectroscopic techniques. These methods are indispensable for examining the electronic structure, chemical composition, and dynamic behaviour of materials across diverse applications – from photonics and quantum technologies to energy storage and catalysis. Spectroscopy offers a non-destructive, element-specific, and often time-resolved perspective into the fundamental properties of matter.

Core techniques such as UV-Vis, infrared (IR), Raman, photoluminescence (PL), and fluorescence spectroscopy remain foundational in characterizing optical and vibrational properties. Meanwhile, more advanced methods like X-ray photoelectron spectroscopy (XPS), electron paramagnetic resonance (EPR) soft X-ray and VUV radiation offer deep insights into electronic states, oxidation environments, and molecular structures. These tools are indispensable in studying bulk materials, glasses, thin films, nanomaterials, quantum dots, and hybrid systems.

Our position

The **Laboratory of Spectroscopy** is a state-of-the-art research centre dedicated to the optical, electronic, and magnetic characterization of advanced materials. It is dedicated to the development and application of cutting-edge spectroscopic techniques and methodologies.

Recent advances in data acquisition and computational analysis have transformed spectroscopy into a high-throughput, data-rich discipline. Machine learning and multivariate analysis are increasingly used to interpret complex spectra, identify hidden patterns, and accelerate materials discovery. Our lab actively develops and applies these tools to enhance the precision and efficiency of spectroscopic investigations.

In addition to standard instrumentation, we design and build custom setups tailored to specific research challenges. This flexibility allows us to explore novel materials and phenomena, including those relevant to nonlinear optics (NLO), quantum computing, photovoltaics, and catalysis.

By combining experimental innovation with theoretical modelling and data science, the **Laboratory of Spectroscopy** plays a central role in advancing materials research and enabling next-generation technologies.

Core Capabilities and Instrumentation

The lab is equipped with a comprehensive suite of advanced instruments that enable both steady-state and time-resolved spectroscopic investigations:

- **UV-Vis-NIR spectroscopy:** based on Cary 7000 Spectrophotometer a high-precision instrument for absorption and reflectance measurements in spectral range from 200 to 3300 nm with unprecedented dynamic diapason up to OD 8. Allows to determine linear optical properties of materials and nanostructures in solutions and in solid state like crystals, powders, thin films and in optical fibres.

- **Spectroscopic Ellipsometry**: The Woolam RC2-X/Basic-NIR (spectral range 210 - 1690 nm) spectroscopic ellipsometer offers full Mueller matrix measurement capabilities, precise azimuthal rotation, and temperature control, allowing detailed studies of various complex material systems. Such crucial characteristics for applications of multilayer systems and optical coatings as film thicknesses, and spectra of complex refractive index could be determined.

- **FTIR Spectroscopy**: The Bruker Vertex 80v Fourier-transform infrared (FTIR) spectrometer (spectral range: 10,000–10 cm^{-1}) probes vibrational modes and chemical bonding in organic, inorganic, and hybrid materials. Equipped with a high-resolution microscope and a cryostat, it enables spatially resolved measurements and temperature-dependent studies. This setup is ideal for investigating molecular structure, phase transitions, and chemical composition with high sensitivity and spectral resolution under vacuum conditions.

- **Raman Spectroscopy**: The TriVista CRS Confocal Raman Microscope (TR777) provides high spatial and spectral resolution vibrational analysis for studying crystal structure, internal stress, phonon interactions, and phase transitions. The system is equipped with a confocal microscope, making it ideal for the investigation of thin films, nanowires, and other micro- and nanoscale materials. It features ultra-narrow band notch filters enabling low-frequency Raman measurements down to 10 cm^{-1}, and offers high spectral resolution <0.1 cm^{-1}, allowing precise detection of subtle vibrational features.

Ultrafast Time-Resolved Spectroscopy

- **Femtosecond Wavelength-Tuneable Laser Spectroscopy System**: The Light Conversion PHAROS/ORPHEUS system, used as an excitation source in combination with Time-Correlated Single Photon Counting (TCSPC) by the PicoQuant HydraHarp 400, is a powerful platform for advanced photonics research. This setup enables the investigation of ultrafast carrier dynamics, exciton lifetimes, and other transient phenomena. Its wavelength tunability and high temporal precision make it ideal for studying a wide range of materials and photo-induced processes.

- **Picosecond Wavelength-Tunable Laser Spectroscopy System** (PL2210A-1k-SH-TH+PG403-SH) **with a Streak Camera** (HAMAMATSU C10910-01 with a spectrometer Kymera 328i-B2): The system offers a broad excitation spectral range from 210 to 2600 nm. It is integrated with a high-performance streak camera and a spectrometer, enabling high-resolution time-resolved photoluminescence studies. The streak camera provides time resolution better than 20 ps and operates in the 200–850 nm wavelength range, allowing precise registration of ultrafast optical signals. This setup is particularly suited for scintillator research and the investigation of fast emission dynamics in advanced materials.

Spectroscopy of Nonlinear optical properties of materials

- Spectroscopy of first hyperpolarizability related NLO properties of materials by means of Hyper Rayleigh Scattering and Second Harmonic Generation (Maker fringe and Kurtz powder) is realized in custom built setups based on femtosecond tunable laser system as excitation source.

- Spectroscopy of nonlinear optical phenomena related to the second and higher hyperpolarizability is studied by Polarization-resolved Z-scan, Beam-Deflection and Third Harmonic Generation methods with femtosecond and picosecond tunable laser systems as excitation source.

Defect and Trap State Analysis

- **Electron Paramagnetic Resonance and Optically Detected Magnetic Resonance:** The Bruker Elexsys-II E500 CW EPR spectrometer and the Oxford Instruments SM4000-8 ODMR system are advanced tools for the identification and characterization of paramagnetic defects, impurity centres, and charge trapping mechanisms. The EPR system operates in both X-band and Q-band frequency ranges, offering high versatility for probing a wide range of spin systems. It also includes

CW-ENDOR capabilities in X-band for enhanced resolution of hyperfine interactions. With an absolute sensitivity of 1.0 × 10^9 spins and a magnetic field range up to 17 kG, it enables precise detection and analysis of weak paramagnetic signals in complex materials. The ODMR system supports multiple detection modes, including Photoluminescence-EPR, Recombination Luminescence-EPR, and Magnetic Circular Dichroism-EPR. It is capable of operating across a magnetic field range of 0–8 T, allowing detailed studies of spin-dependent optical transitions and magnetic field effects on luminescence. Together, these systems provide a comprehensive platform for advanced magnetic resonance studies, enabling deep insights into the electronic and spin properties of a wide variety of functional materials.

- **Thermally Optically Stimulated Luminescence Reader**: The Lexsyg Research LMS system from Freiberg Instruments is a versatile luminescence reader equipped with both X-ray and beta (Sr-90) radiation sources, primarily designed for dosimetry applications. It supports the measurement of Thermally Stimulated Luminescence and Optically Stimulated Luminescence glow curves and spectral analysis. This system enables detailed characterization of trap states and charge carrier dynamics, offering valuable insights into thermal stability, recombination processes, and defect-related phenomena in luminescent materials. Its precise control over stimulation and detection parameters makes it a powerful tool for both fundamental research and applied studies in radiation dosimetry and material science.

Surface and Chemical Analysis

- **X-ray Photoelectron Spectroscopy**: The Thermo Fisher ESCALAB Xi system provides high-resolution surface chemical analysis with exceptional sensitivity, enabling detailed investigation of elemental composition, oxidation states, and chemical bonding environments within the top few nanometers at the surface of a material. Equipped with a monatomic and cluster Ar ion gun, it also supports depth profiling, making it ideal for analysing compositional gradients and layered structures in thin films and interfaces.
  Beyond conventional XPS, the system includes **Reflection Electron Energy Loss Spectroscopy** (REELS), which enables analysis of electronic structure, including band gap estimation, surface plasmon excitations, and dielectric properties. This technique complements XPS by offering insights into near-surface electronic transitions and energy loss mechanisms.
  Additionally, the system is equipped with **Ultraviolet Photoelectron Spectroscopy** (UPS), which uses ultraviolet photons to probe the valence band structure, work function, and density of states near the Fermi level. UPS is particularly valuable for studying the electronic properties of semiconductors, metals, and organic materials, especially in optoelectronic, photovoltaic, and surface engineering applications. Together, these integrated techniques form a comprehensive platform for advanced surface and electronic structure characterization, supporting a wide range of materials research and device development efforts.

Future activities

Building on its strong foundation in luminescence research and optical spectroscopy, the **Laboratory of Spectroscopy** aims to expand its research and technological capabilities through the following key initiatives. These efforts will be driven by a commitment to innovation, interdisciplinary collaboration, and the pursuit of real-world impact.

1. **Integration of In Situ and Operando Spectroscopy.** Future efforts will focus on enabling real-time monitoring of materials under operational conditions, particularly for catalytic, electrochemical, and battery systems. This will provide insights into dynamic changes in electronic and structural properties.

2. **Expansion of Synchrotron Collaborations.** The lab plans to deepen its partnerships with synchrotron facilities such as MAX IV and DESY, while also establishing new collaborations with emerging light sources across Europe. These efforts will ensure continued access to cutting-edge instrumentation not available in standard laboratories.

3. **Exploration of Quantum Materials and Nanostructures.** Research will increasingly target low-dimensional and quantum-confined systems, including 2D materials, perovskites, and quantum dots, with a focus on their optical and electronic behaviour under extreme conditions.

4. **Development of Optical Sensors and Functional Devices.** The laboratory will pursue the design and fabrication of novel optical sensors based on luminescent and photoactive materials. These sensors will be tailored for applications in environmental monitoring, biomedical diagnostics, and industrial process control.

5. **Implementation of Machine Learning for Spectral Analysis.** The lab will adopt data-driven approaches to enhance the interpretation of complex spectroscopic data, enabling faster and more accurate identification of material properties and behaviours.

6. **Exploration of New Application Areas.** In parallel with fundamental research, the lab will actively seek interdisciplinary collaborations to apply spectroscopic techniques in emerging fields such as cultural heritage preservation, space science, and smart materials.

7. **Education, Training, and Public Outreach.** The laboratory is committed to fostering scientific literacy and developing human capital through comprehensive education and training programs. This includes mentoring students and early-career researchers, organizing workshops and summer schools, and participating in international exchange initiatives. Public outreach activities – such as science communication events, open lab days, and collaborations with schools – will be expanded to engage broader audiences and highlight the societal relevance of spectroscopy.

Networking

To access high-resolution analytical capabilities otherwise unavailable in standard laboratory settings, the Laboratory of Spectroscopy maintains active collaborations with leading synchrotron radiation facilities, including **MAX IV** (Lund) and **DESY** (Hamburg). These partnerships enable the use of cutting-edge soft X-ray and vacuum ultraviolet (VUV) radiation for the excitation of luminescence, as well as for detailed analysis of luminescence spectra and decay kinetics. These partnerships significantly expand the lab's analytical capabilities and support frontier research in quantum materials, nanostructures, and functional interfaces.

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THIN FILM AND COATING TECHNOLOGIES

State of the art

The global thin film and coating technologies market is projected to experience robust growth over the next several years, driven by advances in various industries such as electronics, automotive, medical devices, solar energy and glass industry including smart windows. By 2030, the thin film coatings market is expected to reach a value between $17 billion to over $40 billion, growing at a compound annual growth rate (CAGR) of around 5% to 5.4% depending on the specific segment and application [1]. Technological advancements such as Physical Vapor Deposition (PVD), Chemical Vapor Deposition (CVD), and Atomic Layer Deposition (ALD) are also shaping the industry. PVD holds a dominant share due to its versatility and cost-effectiveness, while CVD and ALD are gaining popularity for their precision in advanced applications like semiconductors. These technologies are considered as Green Nanotechnologies [2] and essential in enhancing the performance of optical, electronic, and photovoltaic devices, owing to their superior electrical, optical, and chemical properties.

The coatings find critical applications in various fields, from smart windows and solar cells to advanced sensors in emerging 5G communications, underscoring their importance in both energy efficiency and technological innovation. The European Union's commitment to achieving climate neutrality by 2050 highlights the role of thin films in supporting global sustainability goals [3]. Despite the anticipated growth, the market faces challenges, including the relatively low efficiency of thin film materials and the fragmented use of individual materials in production.

Smart windows represent a transformative innovation in the quest for energy-efficient buildings, particularly in their ability to adapt to varying environmental conditions [4]. Traditional windows, which are static in nature, cannot dynamically adjust their optical properties, limiting their efficiency to specific seasons. This has led to the exploration of chromogenic materials, particularly those that exhibit reversible colour changes in response to external stimuli such as temperature (thermochromic) or light (photochromic). These materials allow the development of smart windows that can automatically regulate light and heat transmission, significantly enhancing energy savings [5]. Current state-of-the-art smart windows often rely on electrochromic devices, which, while effective, are complex and costly due to their multi-layered construction involving electrodes, electrolytes, and electrochromic films. This complexity has impeded their widespread adoption. In contrast, smart windows utilizing photochromic materials offer a more accessible and passive alternative. These windows are activated by solar light, functioning without the need for electricity or external control systems, thus simplifying their design and reducing costs. By automatically adjusting to environmental changes without human intervention, photochromic - thermochromic smart windows hold the potential to revolutionize building efficiency, offering a practical and cost-effective solution for reducing energy consumption across diverse climates and conditions.

Antimicrobial resistance and healthcare-associated infections (HAIs) are critical public health challenges, with HAIs affecting approximately 9 million people annually in Europe [6]. As the effectiveness of antibiotics diminishes, new strategies are urgently needed to reduce HAIs, particularly in clinical settings where high-traffic surfaces are hotspots for pathogen transmission. One promising approach is the application of antimicrobial coatings to surfaces prone to contamination [7]. These coatings, often termed antibacterial or antimicrobial surfaces, can prevent pathogens from attaching to surfaces or kill them upon contact.

Our position

With over 35 years of experience in vacuum deposition thin-film technologies and a well-equipped facility featuring advanced instruments and various characterization methods, ISSP UL has become a recognized centre of excellence for thin-film nanotechnologies in the Baltic region. This expertise significantly contributes to achieving Sustainable Development Goals, European targets for Clean Energy for all Europeans, the Smart Specialisation Strategy of Latvia, and contribute to the European Research Area.

Thin Films Laboratory (TFL) primarily focuses on the deposition of a diverse range of inorganic materials using various deposition techniques – magnetron sputtering, including High Power Impulse Magnetron Sputtering (HiPIMS), thermal and e-beam evaporation, Pulsed Laser Deposition (PLD), Metal Organic Chemical Vapour Deposition (MOCVD), and Atomic Layer Deposition (ALD). The laboratory's current scientific projects are dedicated to the development of novel smart materials and coatings. A list of selected publications and patents related to this activity is given below [8-23].

Recently, TFL has developed deposition method and conducted comprehensive studies on photochromic oxygen-containing yttrium hydride (YHO) [8-10], metastable yttrium monoxide (YO) [11,12], rhenium trioxide (ReO3) with metallic conductivity [13], layered WO3/ReO3, and mixed ReO3-WO3 [14] films. Notably, the photochromic contrast has improved from 40% with YHO alone to 55% in the two-layered structure of YHO/MoO3 [15] under specific measurement conditions. The advanced photochromic properties of YHO forms the basis for further research. The TFL team was recognized by the Latvian Academy of Sciences in 2023 for their outstanding achievements in applied science. The team demonstrated a notable photochromic effect, light-induced resistivity changes at room temperature and ambient pressure, and a superconducting filament effect in YHO and yttrium hydrides [16]. A roll-to-roll

(R2R) system for large-area coatings will be installed at ISSP UL and will primarily be used for developing chromogenic film deposition via magnetron sputtering.

HiPIMS offers significant potential for creating films with superior morphology, density, and smoothness, far surpassing those of conventional DC sputtering technologies. Recent developments include HiPIMS deposition technologies for aluminum-doped zinc oxide [17] and rhenium oxide films with varying rhenium oxidation states [18,19]. The antimicrobial properties of transparent and conductive WO3/Cu/WO3 [20,21] and ZnO/Cu/ZnO [22] coatings have been demonstrated, with improved stability of these properties achieved. The TFL has developed a deposition method at cryogenic temperatures to obtain metastable phases, such as amorphous ZnO-ZnO_2 [23]. The SAF25/50 R&D cluster plant (installed 2015, upgraded 2019) is a multifunctional, expandable, modular, and flexible system designed for the development of thin-film technologies. The plant includes an input/output chamber with an ion gun, a central substrate transfer chamber with a radial telescopic transport arm, and up to seven deposition chambers (thermal and e-beam evaporation, and magnetron sputtering) connected to the glovebox.

Future activities

The future research directions of the TFL will be closely aligned with recent trends in the European research area, as summarized in the Strategy Report and Roadmap developed by the European Strategy Forum ("Vision and Roadmap for European Raw Materials"). These activities will be in compliance with several goals and RIS3 priorities. The research will leverage the available ISSP UL clean room and thin-film facilities, in strong collaboration with industrial partners in Latvia and across the EU.

The "Smart Windows for Zero Energy Buildings" (SWEB 2023-2027) project (www.swebwindow.eu), led by the ISSP UL, is a significant research initiative under the Horizon Europe program, with a budget of €2.4 million. Over the next five years, SWEB aims to develop cutting-edge smart window (SW) technologies, materials, and products that contribute to the growth of zero-energy buildings, addressing EU-wide climate challenges. ISSP, a leader in Functional Materials and Coating research in Latvia, will focus on the development of advanced chromogenic materials – such as photochromic, thermochromic, and electrochromic films – using scalable, cost-effective deposition techniques. The project seeks to build a world-class research team by merging existing expertise at ISSP with new knowledge, particularly in the areas of chromogenic SW materials and technology transfer. This collaboration will not only enhance the research excellence and global visibility of ISSP but also support the broader European Research Area (ERA) by fostering innovation and industry-academic partnerships. Ultimately, SWEB aims to drive the EU towards sustainable zero-energy buildings, smart cities, and smart villages, contributing to long-term environmental goals and the EU's innovation capacity. Rare-earth oxyhydrides (REHO), specifically thin films of yttrium oxyhydride (YHO), a colour-neutral photochromic effect, making them promising for glazing applications. YHO films demonstrate high transmittance in the visible spectrum and can undergo significant photochromic darkening when exposed to solar light, achieving a contrast of 30-50%. These films can be produced using scalable methods suitable for the industry. Based on the study of existing literature, no other family of photochromic materials is able to combine all these desirable properties. However, challenges remain, including the need to optimize photochromic properties, a limited understanding of the photochromic mechanism, and degradation caused by humidity. The TFL proposes to address these issues by producing and studying RE-doped YHO films and multilayer coatings, including large-area coatings on polymer substrates produced using the R2R process.

The TFL aims to develop sustainable, non-toxic antibacterial coatings suitable for large-scale production. This involves exploring eco-friendly alternatives to traditional antibacterial agents, focusing on materials like TiO_2, WO_3, and ZnO, which generate reactive oxygen species (ROS) under UVA or blue light. TFL planning to develop functional multilayer metal oxide (MO) coatings capable of eliminating bacteria and preventing biofilm formation. The innovation lies in the use of ion-assisted techniques and magnetron sputtering, which allow large-scale production, low deposition temperatures, and surface modification. The goal is to optimize lab-scale deposition technologies for large-scale applications using R2R technology.

Roll-to-roll (R2R) PVD magnetron deposition is an advanced manufacturing technique widely used in industries for creating thin films on flexible substrates. The R2R magnetron sputtering machine FHR RC-200-3 (GMBH) will be installed at ISSP UL in 2024. The R2R systems are designed for **continuous, large-scale production** of thin films on flexible substrates, such as polymers, metals, or foils. These systems are crucial for applications in **electronics, energy storage (e.g., flexible batteries), sensors, photovoltaics and smart windows**. R2R PVD magnetron deposition technology is advancing the production of flexible batteries by enabling the deposition of electrodes, barrier layers, and electrolytes on flexible substrates.

Networking

Latvia:

- Sidrabe Vacuum;
- GroGlass;
- KEEP EU;
- RD ALFA Microelectronics;
- AGL Technologies.

Abroad

- Stockholm, Royal Institute of Technology (KTH);
- Stockholm, RISE - Research Institutes of Sweden;
- Department of Engineering Sciences, Uppsala University;
- Fondazione Bruno Kessler, Centre for Materials;
- Germany, Fraunhofer Institute or Surface Engineering and Thin Films IST Braunschweig,;
- Norway, Institute for Energy Technology (IFE).

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MORPHOLOGY AND STRUCTURE

State of the art

In recent decades, material research has increasingly focused on nano-sized and nanostructured materials and devices. Consequently, high-resolution imaging and analytical measurement systems operating at these critical scales are essential for advancing new materials and technologies. Techniques like electron microscopy (EM) and atomic force microscopy (AFM) remain fundamental in characterizing nanomaterials, structures, and devices. Since its inception, EM has improved resolution dramatically—over a 10,000-fold increase in nine decades—enabling sub-Ångstrom-scale imaging with standard laboratory equipment.

While the pursuit of higher resolution has slowed, efforts now emphasize enhancing microscopy systems' versatility. Innovations include integrating spectroscopic techniques, developing advanced detectors, and refining in situ capabilities such as heating, cooling, and electrical biasing. These developments have enabled breakthroughs in studying challenging materials, including soft matter, biological samples, 2D materials, and systems requiring dynamic chemical and structural analysis.

Currently, computational microscopy is gaining prominence, driven by increased computational power and the vast data from ultra-fast detectors. Machine learning is improving image acquisition, automating data analysis, and enabling sample reconstruction from large datasets. Such methods, combining imaging with analytical techniques, are increasingly used to enhance accuracy and efficiency.

The Microscopy Laboratory focuses on advanced measurement techniques, developing cutting-edge microscopy methodologies to push the boundaries of material science research. Alongside specialized measurements, we prototype and create custom setups for unique research needs, contributing to both discovery and practical applications.

Parallel to advances in EM, other analytical methods have become routine in material studies, focusing on chemical composition. Notable examples include EDS (Energy Dispersive X-ray Spectroscopy), WDS (Wavelength Dispersive X-ray Spectroscopy), EELS (Electron Energy Loss Spectroscopy), XPS (X-ray Photoelectron Spectroscopy), ToF-SIMS (Time-of-Flight Secondary Ion Mass Spectrometry), and XRD (X-ray Diffractometry). These methods, often paired with microscopy images, provide detailed insights into sample homogeneity, composition, and structure.

Modern microscopy systems now extend beyond imaging and analysis to include nanoscale manipulation. Advanced electron and ion microscopy systems, like SEM-FIB (Scanning Electron Microscopy-Focused Ion Beam), equipped with nano-manipulators, gas injection systems, and precision tools, enable nanofabrication alongside in situ electrical and optical measurements. These platforms facilitate rapid prototyping and testing of novel nanoscale devices, accelerating R&D processes. Additionally, SEM-FIB systems play a crucial role in specimen preparation for volumetric studies, enabling precise cross-sectioning and 3D reconstruction via slice-and-view techniques..

Our position

Microscopy laboratory was established in 2020. It focuses on the study of materials structure, morphology and composition, by using modern experimental and theoretical methods. This is a method-based laboratory, which provides services to other research laboratories.

The laboratory has four main pillars: electron microscopy imaging and spectroscopy (I), X-ray and electron diffraction methods (II), microhardness and nanoindentation methods (III) and atomic force microscopy (IV).

I. Electron microscopy is a relatively new direction at ISSP UL; however, a significant effort has been involved to obtain the expertise in this field. This has led to multiple research publications already each year electron microscopy contributing to around 30 research papers. In the past 10 years, three SEMs and one TEM were acquired. The newest addition is a state of the art SEM-FIB system Helios G5 UX. This microscope is equipped with a variety of detectors and add-ons (EBSD and EDS) allowing high-level analysis. Contrary to the conventional SEM systems, this one enables analysis and visualization not only of the specimen's surface, but volume as well and can be used for 3D reconstruction of material [1]. In addition, all measurements can be performed at low acceleration voltage with super-high resolution: 0.7 nm at 1 kV for SEM and 2.5 nm at 30 kV for FIB. The high resolution and low voltages of ion beam column allows high quality lamella preparation even for challenging materials like polymers and porous nanostructured ceramics and thin films [2-4]. Focused ion beam system has been used to fabricate non-standard experimental vacuum trinode microelectronic device, which shows potential of using FIB not only for sample preparation, but also in prototype device fabrication [5]. Additionally, in-house computer script permits easier correllative microscopy between SEM and other instruments [6]. The other installed SEM-FIB system, Tescan Lyra is tailored to perform non-conventional studies right in the microscope, such as electrical, optical and force measurements. It is equipped with 5 nano-manipulators for *in situ* measurements and prototyping. Recently this instrument has been employed for *in situ* study showing in real time electromechanical resonance of Ga_2O_3 nanowires [7]. Both SEM-FIB systems are equipped with electrical and optical inputs for in-situ electrical and optical properties measurements.

II. X-ray diffraction (XRD) is one of the most used characterization methods at ISSP UL. As with most characterization methods, the analysis of the results is as important as the acquisition itself; therefore, the laboratory maintains access to the newest databases and has experience in efficient application of them. Two instruments are in active use: PANalytical X'Pert PRO and Rigaku MiniFlex Benchtop X-Ray diffractometer. X'Pert PRO device (max. 2.2 kW, 60 kV) can be used to provide high-resolution powder diffraction data, phase identification and quantitative phase analysis, analysis of thin films and coatings, crystallite size and strain determination, as well as has the ability to perform kinetic and non-ambient experiments. In addition, highly controlled in situ XRD measurements in temperature range from -170 to +450 °C can be performed. At the moment the system has been *in-house* modified so that the simultaneous heating/cooling, electric characterization or electric biasing experiments can be done while also getting insights into crystal lattice dynamics, this addition is very recent, and the articles are in the preparation stage. The second XRD device (MiniFlex benchtop X-ray diffractometer) is a multipurpose powder diffraction instrument used for rapid phase identification and quantitative phase analysis offering easy and fast sample loading and unloading, which is highly beneficial with large sample series and in industrial research.

Advanced XRD analysis of the results is available: Rietveld refinements of the XRD data are used to analyze X-ray diffraction data by fitting experimentally obtained spectra with theoretical models. Rietveld method is used to determine the phase distribution, sizes and shapes of crystallites and bond lengths of the material, as well as to identify structural defects and to solve crystal structure of the powder sample. The XRD data analysis can be used in combination with electron diffraction measurements done in TEM (SADP) and SEM (EBSD) and has been compared with the results obtained by EXAFS spectroscopy [8], showing reliability of the XRD machine and Rietveld refinement technique even on a laboratory based instrument.

III. Surface properties of samples are essential for many fields and applications and can be studied using advanced techniques like microhardness testing and nanoindentation. Our laboratory team has decades of expertise in these methods and operates a modern, high-precision nanoindentation system (Agilent G200) for detailed surface characterization. This setup allows us to accurately measure mechanical properties such as hardness, elastic modulus, and wear resistance at micro and nanoscale levels, making it valuable for research in materials science, engineering, and nanotechnology as demonstrated on diamond-like thin films [9]. Our facility is equipped to handle a broad range of materials, ensuring high-quality, reliable measurements for diverse applications.

IV. Atomic force microscopy (AFM) nowadays is used only for very specific studies of samples. Despite that, the researchers from the laboratory successfully apply this technique to various materials and structures, as reflected in published results. With the expansion of the laboratory, purchase of new hardware for AFM is being considered to replace outdated instruments. Looking ahead, we plan to further expand our capabilities by acquiring a state-of-the-art Atomic Force Microscope (AFM) with a variety of spectroscopy modes. This will enable us to perform even more comprehensive surface analysis, including mechanical, electrical, and chemical property measurements at the nanoscale, complementing our existing expertise in microhardness and nanoindentation. Recently AFM was used to investigate adhesive properties of gold nanorods/nanoparticles on Si surface [6].

Scientific output in form of publications is accompanied by the fulfilment of multiple industry contracts, and laboratory provides services for third parties.

Future activities

The top priority for the laboratory is to continue providing high-quality support to other laboratories within the Institute, while also addressing the needs of industry. As a method-based support laboratory, our strategic development will focus on modern characterization techniques. Two parallel development threads will guide our growth: advancing instrumentation and refining analytical methods.

Instrumentation and Methods. To enhance our capabilities, the laboratory aims to expand the use of correlative microscopy, integrating multiple characterization techniques to analyze materials at various length scales. This includes the adoption of in situ microscopy, which allows real-time observation of materials under working conditions, providing critical insights for industrial R&D.

Although we already possess a broad range of measurement setups, upgrading and expanding them is crucial. For instance, our current AFM setup, which is limited to imaging, will be enhanced with advanced features such as Conductive Probe AFM, I-V Spectroscopy, Electrostatic Force Microscopy (EFM), Kelvin Probe Force Microscopy (KPFM), Piezoelectric Force Microscopy (PFM), and Scanning Capacitance Microscopy. These methods will significantly improve our ability to conduct extended R&D.

Our state-of-the-art SEM-FIB systems already offer excellent performance, but we plan to add in-situ SEM capabilities, such as "In-SEM" AFM , to enable simultaneous data acquisition from both devices for improved versatility. In addition, we are working on custom integration of optical light detection/injection with SEM imaging, an approach particularly beneficial for photonics-related research.

To further expand our elemental analysis, Time-of-Flight Secondary-Ion Mass Spectrometry (TOF-SIMS) and Wavelength-Dispersive Spectroscopy (WDS) will be added to the SEM-FIB system. These enhancements will provide comprehensive spatial, spectral, and in-volume analysis, enabling full data acquisition within a single system.

In the future, it would be highly beneficial to upgrade our TEM system with Electron Energy Loss Spectroscopy (EELS) detectors or replace it with a next-generation TEM featuring probe correction and a monochromator for enhanced resolution. This upgrade would significantly improve our capabilities in STEM and EELS, allowing for more detailed material analysis and enabling advanced studies in combination with X-ray absorption spectroscopy

Another recent initiative is the introduction of in situ mechanical/electrical/optical/ enviromental A promising initiative is the introduction of in situ mechanical, electrical, optical, and environmental property probing in XRD. This approach enables the correlation of macroscopic material properties with atomic-level changes, providing valuable insights for both fundamental research and industrial applications.

Data Analysis and Machine Learning In addition to hardware upgrades, we are incorporating advanced data analysis methods. Machine learning (ML) and artificial intelligence (AI) will play an increasingly important role in our workflow. ML algorithms will help automate data analysis, identify hidden patterns, and provide deeper insights, while AI can simulate complex systems and optimize R&D processes. These technologies will enhance both the speed and accuracy of our research, supporting more efficient material characterization.

Complementary Methods and Industrial Applications A single technique often cannot provide complete information about a material. Therefore, we employ complementary characterization methods, mapping local chemistry, crystallography, molecular structure, and functional properties. By cross-correlating data from various methods, we gain a deeper understanding of material behavior. Additionally, in situ measurements enable us to study materials and devices under real-world operating conditions, which is highly relevant for industrial R&D. Our goal is to incorporate these modern characterization methods into industrial R&D workflows, providing companies with the critical data they need to overcome technological barriers. The ability to design safe new materials and develop reliable manufacturing processes is key to rapid up-scaling and maintaining high-quality control, a priority for industry leaders.

Networking

As a support laboratory, we actively collaborate with colleagues from various local institutes and international research institutions, as well as industry partners. In fact, approximately half of our publications are the result of these collaborative efforts

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