## 25TH SYMPOSIUM ON PHOTONICS AND OPTICS SPO 2024

# **Report of Contributions**

Type: Oral

### Excitation of Frequency Harmonics of q-Gaussian Laser Beams Propagating through Radially Inhomogenous Plasma Channel

Friday, November 8, 2024 3:15 PM (15 minutes)

We investigate the interplay between self-focusing and higher harmonic generation (HHG) in a pre-formed, collisionless parabolic plasma channel. A *q*-Gaussian laser beam, with its non-uniform intensity profile, induces a ponderomotive force that reshapes the plasma density distribution. This density gradient drives a plasma wave, which interacts with the laser to generate HHG. Using moment theory, we derive a differential equation describing the laser beam's spot size evolution and numerically solve it to explore the influence of laser intensity, wavefront distortion, plasma density, channel depth, and harmonic order on beam propagation and HHG efficiency. Our results provide valuable insights into the underlying mechanisms governing self-focusing and HHG in parabolic plasma channels, paving the way for optimizing HHG sources for applications such as attosecond pulse generation and coherent extreme ultraviolet radiation.

#### Type of presence

Presence online

Primary author: LIMBU, Abhay (Lovely Professional University)
Co-author: Dr GUPTA, Naveen (Lovely Professional University)
Presenter: LIMBU, Abhay (Lovely Professional University)
Session Classification: Laser-Plasma Interactions and Spectroscopy

Type: Oral

### Ion Acoustic Wave Excitation by Bessel Gauss Laser Beams in Plasmas with Axial Density Ramp: Effect of Self Focusing

Friday, November 8, 2024 3:30 PM (15 minutes)

This theoretical study examines the interaction between Bessel-Gauss laser beams and ion acoustic waves (IAWs) in a plasma with a gradually increasing density profile. The focus is on how the laser beams self-focusing affects the power of the generated IAWs. As the laser propagates through the plasma, it excites an IAW at its characteristic frequency. Nonlinear coupling between the IAW and the laser arises due to the ponderomotive force acting on plasma electrons. By employing variational theory and the WKB approximation, we derive semi-analytical solutions for the coupled nonlinear wave equations. Our results demonstrate that the self-focusing of the laser beam plays a crucial role in determining the power of the excited IAW.

#### Type of presence

Presence online

**Primary author:** PRATAP, Rudra (lovely Professional university, Phagwara, Punjab, India)

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Presenter: PRATAP, Rudra (lovely Professional university, Phagwara, Punjab, India)

Session Classification: Laser-Plasma Interactions and Spectroscopy

Type: Oral

## Ultrafast structural changes in Fe studied by time-resolved X-ray diffraction

Monday, November 4, 2024 2:30 PM (15 minutes)

The atomic structure of the thin Fe layer after sub-ps pulsed laser annealing has been studied by time-resolved X-ray diffraction [1]. The laser pulse energy is transferred to the lattice within about 1 ps due to the strong electron-phonon coupling. This rapid heating leads to ultrafast melting. However, solid-solid structural transformations occur below the threshold of complete melting. At high temperatures, phonon softening occurs, leading to lattice distortion, as predicted by ab initio theoretical simulations.

[1] J. Antonowicz et al., Acta Materialia 276 (2024) 120043

#### Type of presence

Presence online

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**Session Classification:** Exploring Ultrafast Phenomena with the XFEL: Instruments, Capabilities, and Applications

Track Classification: USyNC Workshop

Type: Oral

# Synthesis and Optical Characterization of Gd3M2Al3O12: M=Ce+3, Fe+3

Tuesday, November 5, 2024 5:45 PM (15 minutes)

Author: Dewasthali Tejaswi Ramchandra

Co-author: Suman Rani

Garnets have been receiving attention lately considering to their potential to improve the efficiency of photonic devices. As a host, garnets have exceptional chemical and physical stability, which makes them dependable options for a range of applications in materials science, electronics, and optics. This work examines the structural and optical characteristics of two cubic garnets, Gd3Ce2Al3O12 (GCAG) and Gd3Fe2Al3O12 (GFAG), through their synthesis using the solgel method (sintered at 11000C for GCAG and 9500C for GFAG). The microstructural properties were investigated using FTIR spectroscopy. The band gap was determined to be 3.73 eV for GCAG and 2.63eV for GFAG using UV-Vis spectroscopy. Intriguing optical characteristics of GCAG and GFAG are demonstrated by multicolour emission in their Down conversion (DC) emission spectra.

#### Type of presence

Presence online

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Presenter: Ms TEJASWI RAMCHANDRA, Dewasthali (Lovely Professional University Punjab)

Session Classification: Workshop on Sustainable Materials and Technologies

Type: Oral

### Enhancing Optical and Electrical Performance of ZnO Thin Films by Mg dopant

Tuesday, November 5, 2024 6:00 PM (15 minutes)

Author: Shruti Bakshi

Co-Author: Suman Rani

Transparent conductive materials that are conducted and transmissive are an important aspect in the field of optics and electronics as they play a major role in modern optoelectronic devices. Zn1xMgxO (x = 0.01) thin films are such material that lies in the category of Transparent conducting materials exhibiting exciting properties like low absorption of light, and high transmission. The study's objective is to analyze the influence of Mg doping on pure ZnO thin films formed on a glass substrate by the sol-gel spin coating approach annealed at 500°C for five hours. According to the X-ray diffraction study, the films showed a maximum intensity hexagonal wurtzite structure in the (1 0 1) plane. As the Mg doping concentration increased, the diffraction peaks reduced. Optical properties indicate transmittance, absorbance, reflection, refractive index, extinction coefficient, and optical band gap. By increasing Mg doping, optical examination revealed a considerable increase in transmittance from 82.7 to 88.7 % in the visible region. Also, the energy band gap values reduce from 3.25 eV to 3.14eV because of the s-d and p-d exchange interactions. When the concentration of magnesium in ZnO increases, there is a trend toward an increase in both the mobility and electrical conductivity of the magnesium-doped thin films. The excellent optical and electrical properties confirm that Mg-doped ZnO thin films are promising candidates for transparent conducting oxide applications.

#### Type of presence

Presence online

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Session Classification: Workshop on Sustainable Materials and Technologies

Type: Poster

### Nonlinear Spatial Frequency Chirping Of Quadruple Gaussian Laser Beams Interacting with Narrowband Gap Semiconductors: Effect of Self Focusing

Friday, November 8, 2024 4:51 PM (4 minutes)

Nonlinear Spatial Frequency Chirping Of Quadruple Gaussian Laser Beams Interacting with Narrowband Gap Semiconductors: Effect of Self Focusing

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Abstract

This paper investigates the nonlinear spatial frequency chirping (NSFC) of quadruple Gaussian (QG) laser beams interacting with narrowband gap semiconductors. The study focuses on the influence of self-focusing, a nonlinear optical phenomenon that can significantly alter the beam's propagation characteristics. The nonlinear Schrodinger equation (NLSE) is employed to model the beam propagation, incorporating the effects of self focusing. Numerical simulations are conducted to analyze the NSFC behavior under various conditions, including different beam intensities, semiconductor bandgaps, and initial beam profiles. The results demonstrate that self-focusing plays a crucial role in enhancing the NSFC effect, leading to a more pronounced spatial frequency spread. Additionally, the paper explores the impact of semiconductor bandgap on the NSFC, revealing that materials with narrower bandgaps exhibit stronger nonlinear interactions and consequently more significant NSFC. Overall, this study provides valuable insights into the nonlinear optical properties of quadruple Gaussian laser beams in narrowband gap semiconductors and highlights the importance of considering self-focusing in understanding the NSFC phenomenon.

#### Type of presence

Presence online

Primary author: MALIK, Nishu (Lovely Professional University Phagwara)Presenter: MALIK, Nishu (Lovely Professional University Phagwara)Session Classification: Poster Session

Type: Poster

### Recovery of germanium optical elements for infrared technique devices

Friday, November 8, 2024 4:00 PM (3 minutes)

Germanium optical elements are widely used as passive components (lenses, prisms, windows, protective screens) of the great majority of infrared devices. During operation, especially under extreme conditions, such elements frequently suffer mechanical damage or lose transparency resulting from the degradation of anti-reflective coatings.

The report presents the results of physical-technological and chemical-technological research aimed at the development of methods for removing anti-reflective coatings from the surface of germanium optical elements and their subsequent removal from the coating layer. The material of antireflective coatings, which penetrates into the near-surface layer of the optical elements during their manufacture and operation, makes it impossible to restore the optical elements.

The results of the development of etchant composition as well as of the technological regimes of removing the material of anti-reflective coatings from the surface and near-surface layer of optical elements are given. A technique for determining the concentration of impurities in optical elements after removing the anti-reflective coating has been developed. The results of the approbation of the developed technique show that it allows determining the concentration of electrically active impurities at the level of  $(5-7) \times 1013$  cm–3.

Germanium optical elements, cleaned of anti-reflective coating by the proposed technical method, can be used both for repeated application of new anti-reflective coatings with their further use in infrared technology, and for processing into raw materials for growing germanium optical crystals without the use of rectification refining methods.

The work was carried out within the framework of the project № 173/0010 "Development of the technology for restoration of germanium optical elements of thermal imaging devices for the repair of armored and aviation equipment" of National Research Foundation of Ukraine.

#### Type of presence

Presence at Taras Shevchenko National University

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#### Session Classification: Poster Session

Type: Invited Talk

## The effect of substrate temperature in laser-induced high velocity micro-particle impacts

Thursday, November 7, 2024 11:30 AM (25 minutes)

The impact of microscale particles with a surface is of fundamental importance in surface coating technologies such as laser-induced forward transfer or cold spray. Successful bonding between the particles and the substrate requires impact velocities higher than the so-called critical adhesion velocity. Previous experimental and theoretical results showed that the critical velocity is a function of numerous factors. Among them, the substrate temperature is important since substrate deformation and rupture of the oxide on the substrate through such deformation are critical to forming metallurgical bonds with the particle. Herein we conducted single-particle impacts on a variable-temperature substrate for three systems (Al–Al, Sn–Sn, and Ti–Ti) with particles individually selected within a narrow size distribution. The experimental investigations were carried out using an in-house-designed all- optical platform known as laser-induced particle impact test (LIPIT).

Our results show a downward shift of the critical velocity for each material combination, by a significant amount, which we attribute to the lower dynamic strength of the thermally softened substrate. Our experimental results are in good agreement with numerical simulations, where we predict the dependence of bonding window and the critical velocity in function of substrate temperature. The results support literature trends that a higher substrate temperature can compensate for a lower particle velocity, which may speak to improved procedures for particle deposition in cold spray or laser-induced forward transfer technology.

#### Type of presence

Presence online

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Session Classification: Advances in Nonlinear Optics and Laser-Matter Interactions

Type: Invited Talk

## Hard X-ray Photoelectron Spectroscopy at DESY

Monday, November 4, 2024 3:00 PM (30 minutes)

Photoelectron spectroscopy using excitation by hard X-rays in the range of 2.5-10 keV (HAXPES) is rapidly developing at synchrotron light sources worldwide. Its comparatively large probing depth (10-30 nm) makes it a powerful tool for the study of complex materials, magnetic (buried) nanostructures, device-like structures, and catalytic interfaces.

The P22 beamline at PETRA III is a cutting-edge facility dedicated to HAXPES techniques, featuring four specialized experimental end stations for high-resolution studies of the electronic structure of solids. These instruments are fully operational and used in close collaboration with external user groups, reflecting the wide range of scientific fields engaged by the P22 beamline community. The P22 beamline first received light in November 2017 and conducted its first user experiments in June 2018. Since then, it has contributed to over 100 publications. Access to P22 is granted through a rolling review process, with accelerated turnover times as short as two months. Users from Ukrainian universities can receive full travel reimbursement under the new EU program NEPHEWS.

This contribution provides a concise overview of the experimental capabilities of the P22 beamline and highlights the most prominent scientific results from the HAXPES end station.

#### Type of presence

Presence online

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Presenter: Dr GLOSKOVSKII, Andrei (Photon Science / DESY)

**Session Classification:** Advanced Luminescence and Spectroscopy Techniques at DESY: Instruments, Materials, and Applications

Track Classification: USyNC Workshop

Type: Poster

### Gouy Phase Shift of Bessel Gauss Laser Beams in Plasmas with Axial Temperature Ramp: Effect of Self Focusing

Friday, November 8, 2024 4:58 PM (3 minutes)

This paper investigates the Gouy phase shift of Bessel-Gauss laser beams propagating through a plasma medium characterized by an axial temperature gradient. The interplay between the Bessel-Gauss beam profile and the self-focusing effect induced by the plasma is examined. The analytical expression for the Gouy phase shift is derived, incorporating the influence of both the beam's spatial structure and the plasma's temperature distribution.

Variational theory has been used to make predictions of the impact of self-focusing on the Gouy phase shift. The results demonstrate that the axial temperature ramp significantly modifies the Gouy phase shift, leading to deviations from the behavior observed in uniform plasma environments. The findings have implications for various applications involving laser-plasma interactions, including plasma diagnostics, laser-driven particle acceleration, and high-harmonic generation.

#### Type of presence

Presence online

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Presenter: BRAR, Rajnoor Singh (Lovely Professional University)

Session Classification: Poster Session

Type: Invited Talk

### 2-dimensional MoS2 for photonic applications

Tuesday, November 5, 2024 12:40 PM (20 minutes)

Two-dimensional molybdenum disulfide (MoS2) has attracted significant interest in the field of optoelectronics owing to its direct bandgap, tunable optical properties and the potential for realizing van der Waals heterostructures. It is considered one of the most successful transition metal dichalcogenides, thanks to its exceptional mechanical, electronic, optical, and transport properties that may allow for future radical innovation breakthroughs in different applications [1]. The potential is particular high for light-based applications, thanks to its tunable direct gap in the 1.6 - 1.9 eV range. In this talk, I will provide a comprehensive overview of: i) fundamental properties of 2D-MoS2, ii) the main characterization techniques used to study this material, iii) the preparation by chemical vapour deposition (CVD) of 2D MoS2. Among various methods, chemical vapour deposition is considered an excellent candidate thanks to its simplicity, widespread use, and compatibility with other processes used to deposit other semiconductors [2].

Then, I will give a brief overview of the latest developments in light-based devices leveraging MoS2, including photodetectors, phototransistors, waveguides and optical cavities with integrated 2D-MoS2 and single photon sources [3]. By summarizing such recent achievements, I will provide some insights into the high potential offered by this 2D material in photonics.

[1] Yazyev, O. V.; Kis, A. Mater. Today 2015, 18, 20-30.

[2] Seravalli, L.; Bosi, M. Materials. 2021, 14, 7590.

[3] Esposito, F.,Attolini G; Bosi M.; Seravalli, L.; Semiconductor Physics, Quantum Electronics & Optoelectronics (to be published)

#### Type of presence

Presence online

Primary author: Dr SERAVALLI, Luca (IMEM-CNR Institute)

**Presenter:** Dr SERAVALLI, Luca (IMEM-CNR Institute)

Session Classification: Workshop on Sustainable Materials and Technologies

Track Classification: Workshop on Sustainable Materials and Technologies

Type: Invited Talk

### The luminescence of aluminate spinels: overview and application to dosimetry

Tuesday, November 5, 2024 3:35 PM (30 minutes)

Spinels present large compositional diversity and property tunability and thus are of interest to many technology fields. The cubic structure and broad optical transparency associated with a large band gap of the Mg and Zn aluminate spinels make these materials particularly attractive for optical applications.

MgAl2O4 and ZnAl2O4 in a diversity of forms, from powders prepared by the co-precipitation method and calcined at 900 C for 2 hrs. in air to natural crystals and artificial crystals grown by the Czochralski method, were investigated. Structural characterization was executed by X-ray diffraction and Raman spectroscopy. Radioluminescence (RL) under X-ray excitation from room temperature to 400 C was recorded. RL measurements revealed that both spinels presented a broad band peaked at ~400 nm together with other bands attributed to Cr3+, Mn4+ and Mn2+ impurities. Thermoluminescence (TL) spectroscopy measurements up to 400 C were executed towards the identification of the recombination centers involved in the TL process, with the glow curves presenting several overlapping bands. TL spectroscopy measurements showed TL signal to be originated mostly from Cr3+ impurities. The stability of TL signal storage (fading) was also evaluated. Optically stimulated luminescence (OSL) was characterized as a function of the irradiation dose and in terms of its signal linearity with the irradiation dose and reproducibility. The minimum detectable dose (MDD) was determined, the OSL decay curves were analyzed in terms exponential functions, and fading was evaluated. A critical evaluation of MgAl2O4 as an OSL dosimeter is presented.

#### Type of presence

Presence online

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Presenter: Prof. JACOBSOHN, Luiz (Clemson University)

Session Classification: Workshop on Sustainable Materials and Technologies

Track Classification: Workshop on Sustainable Materials and Technologies

Type: Invited Talk

### Optical transparency windows in near-infrared and short-wave infrared for skin, skull and brain: tissue optical properties and fluorescence bioimaging

Friday, November 8, 2024 2:00 PM (20 minutes)

Fluorescence imaging is a perspective noninvasive optical technique to visualize emitting molecules and nanomaterials in biological objects. The limitation of this method is a depth of imaging due to a strong attenuation of light by the tissue, however, the use of near-infrared (NIR) irradiation allows for the visualization of objects under the tissue surface for millimeters. The tissue transparency windows within  $^{700-1000}$  nm (NIR-I) and 1000-1350 nm (NIR-II) are conventional. Moreover, the lately explored short-wave IR (SWIR) optical transparency windows ranging  $^{1550}$  to 1870 nm (SWIR or NIR-III, NIR-IIb) and  $^{2100}$  to 2300 nm (SWIR-II) have more advantages due to much lower light scattering by turbid tissues. They are related to the attenuation coefficient and total attenuation length are determined for all windows and tissue types. The spectra indicate transmittance peaks in NIR, NIR-II and SWIR-II, with maximum tissue permeability for SWIR light. Thus, when comparing IR fluorescence imaging of quantum dots emitting at  $^{1.0}$ , 1.3 and 1.6 µm through the scalp skin, skull bone and brain, the SWIR fluorescence is detected the best. Moreover, it shows the utmost enhancement for the skull, which is a highly scattered medium. The benefits of the NIR-II and SWIR windows are shown for IR fluorescence imaging, the technique where the collimated transmission component is more important than the diffused one.

#### Type of presence

Presence online

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Session Classification: Biomedical Imaging and Nanotechnology

Type: Oral

### Transitioning from Manual to Automated Control: Mode-Locked Ultra-Fast Fiber Lasers via Machine Learning and Genetic Algorithms

Thursday, November 7, 2024 2:45 PM (15 minutes)

Mid or Near-IR Mode-Locked Lasers offer several advantages over simple Continuous-Wave (CW) Lasers due to their unique operational characteristics and significant commercial applications. Mode-locked lasers typically generate ultra-short and ultra-fast pulses with very high peak powers and repetition frequencies, which are essential for a wide range of applications such as nonlinear optical processes, high-resolution imaging, precision material processing, micro/nanomachining, optical coherence tomography (OCT), and frequency comb generation.

In CW lasers, the amplification of light through stimulated emission is easier for longer wavelengths, making it more challenging to generate high-frequency lasers. Mode-locked lasers, on the other hand, offer advantages in these areas but come with increased complexity in their design, construction, and operation. A key challenge is achieving and maintaining precise cavity alignment, which is crucial for ensuring stability in this highly complex nonlinear optical system. Traditional methods, such as the Split-Step Fourier Method (SSFM), rely on compact numerical calculations and multiple trial experiments. However, these conventional approaches often face limitations when confronted with the intricate challenges of achieving stable mode-locking.

Artificial Intelligence (AI), an emerging technology centered around data-driven analysis, offers new perspectives on improving the stability of mode-locked lasers. This research article explores the integration of a feedback controller-based fast controller with the Genetic Algorithm of Machine Learning, aiming to achieve stable ultra-fast and ultra-short pulses in the shortest possible time through an automatic mode-locking process. The inclusion of AI accelerates the convergence of optimal solutions, reducing the time and complexity required for manual cavity adjustments, thus paving the way for more efficient and scalable laser technologies.

#### Type of presence

Presence online

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Session Classification: Advances in Nonlinear Optics and Laser-Matter Interactions

Type: Poster

## Creation of nano-objects for nanoelectronics and spintronics

Friday, November 8, 2024 4:06 PM (3 minutes)

Among the promising and innovative technologies of today, nanoelectromechanical systems, nanoelectronics, and its subdivision - spintronics, occupy a leading place. At the same time, onedimensional structures - nanocontacts and nanowires - are of particular interest, based on which it is possible to form highly efficient nanocircuits with small dimensions and low power consumption. However, during the formation of nanocontacts and nanowires, elastic stresses arise in their structure, which can significantly change the atomic structure and geometry of the wire or contact up to the rupture of the structure, which subsequently leads to a significant change in their mechanical and quantum properties. In addition, the properties of nanowires and nanocontacts formed on various non-magnetic substrates are being actively studied today. A nanowire formed on a substrate is the prototype of a nanoscale electronic circuit, therefore, the study of interactions in the "nanowire-substrate" system is one of the priority areas of nanoelectronics and spintronics. In the presented work, a scanning tunneling microscope, "Micro-nano mode", was used for the non-contact formation of nanorelief on the surface of metal substrates and interelectrode mass transfer with nanometer resolution. The fundamental possibility of non-contact modification of the surface of an indium nanofilm with a tunneling current by creating nano-objects on it was shown. A nano-object as a contact pad was obtained using the single-pass method. The dimensions of the nano-object in the form of a square were 1 µm by 1 µm, and the depth of the created nano-object was about 15 nm. The possibility of creating a group of nano-objects in the form of nanotracks (wires) obtained by modifying the surface non-contact using the two-pass technique was demonstrated. The dimensions of the nano-objects in the form of tracks (wires) were 1.5 µm by 0.4 µm and 1.5 µm by 0.8 µm, respectively, and the depth of the created nano-objects was about 7 nm.

#### Type of presence

Presence online

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Session Classification: Poster Session

Type: Oral

## Enhanced chiral sensing with plasmonic nanostructures

Thursday, November 7, 2024 4:45 PM (15 minutes)

Chirality is used to describe an object that is not superposable on its mirror image. Despite having the same chemical structure, most chiral molecules show significant differences in biological activity, being the poison or the drug depending on the handedness. The main difficulty during the measurement of chiral substances is the need to detect extremely weak chiroptical signals from a small concentration of molecules. In this work, we first excite a surface plasmon-polariton via the prism coupling in the attenuated total internal reflection regime with a plane TM-polarized wave in Kretschmann configuration. In this case, the small response in the TE-polarization emerges due to the mixing of electric and magnetic fields. As a result, there is the angular difference between the spectral resonances in right- and left-handed circular polarized waves due to the presence of chiral substance. To characterize the sensitivity of chiral substance detection we consider the amplitude and phase of the differential reflectance and the dependence of the angular shift on the chiral parameter. We aim to increase the angle of divergence between the reflection spectra peaks for the left- and right-handed circular polarization, and accordingly the efficiency of chiral sensing. It may be achieved via the enhancement of the response in TE polarization. Introducing the efficient anisotropic two-dimensional conducting layer instead of the metal film, we improve the efficiency of chiral sensing by about an order of magnitude.

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#### Type of presence

Presence at Taras Shevchenko National University

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Session Classification: Advances in Metasurfaces and Plasmonic Nanostructures

Type: Invited Talk

# Exciton and trion photoluminescence properties in 2D molybdenum disulfide

Tuesday, November 5, 2024 1:20 PM (20 minutes)

Nanolayers of transition metal dichalcogenides are interesting as 2D materials for novel nanooptoelectronics. Molybdenum disulfide is one of the most studied. At the limit of the monolayer, whose thickness is ~0.7 nm, molybdenum disulfide possesses a direct optical bandgap leading to an intense excitonic photoluminescence (PL) and a bandgap value of about 1.88 eV (660 nm) at room temperature. Its emission spectrum consists of the A and B exciton peaks. The A peak is dominant and, in turn, contains two components related to a neutral exciton and a negative trion. The optical properties of the exciton and trion are dependent of external conditions, i.e., temperature and strain, or various laser excitation conditions, i.e., energy and power. At the same time, the exciton emission is highly dependent on the number of layers: PL redshifts and quenches with increasing thickness. Moreover, the trion properties are highly dependent on these conditions because its binding energy is much less than that of the exciton. The trion spectral weight and dissociation energy are observed to increase with the number of layers, being correlated with an increase in nonequilibrium electron density. A faster intensification of the trion component compared to the A exciton occurs with increasing temperature and excitation power. Also, the intense exciton/trion PL band redshifts and becomes more asymmetric when increasing excitation power. Under strain, the PL undergoes the strain-related blueshift accompanied by a weakening of the contribution of the trion to the spectrum and the trion binding energy.

#### Type of presence

Presence online

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Session Classification: Workshop on Sustainable Materials and Technologies

Track Classification: Workshop on Sustainable Materials and Technologies

Type: Invited Talk

### Stem cells loaded with near-infrared nanoparticles for dynamic imaging of cancer, metastasis and inflammatory focuses

Friday, November 8, 2024 1:40 PM (20 minutes)

Different types of nanoparticles are widely used because they have unique properties which make them suitable for the diagnostics and therapy (theranostics). They can improve detection selectivity and sensitivity, as imaging agents, delivery systems for encapsulated drugs, proteins and nucleic acids. Nanoparticles show high loading capacity, stability, high drug bioavailability and biocompatibility. However, nanoparticles face different biological barriers while entering the body, which limit their successful biodistribution for diseases theranostics. These biological barriers include immune clearance in the liver and spleen, permeation across the endothelium into target tissues, penetration through the tissue interstitium, endocytosis in target cells, diffusion through cytoplasm, and eventually entry into the nucleus. Additionally, there is another important biological barrier in the brain which is called blood brain barrier. To solve the problem of overcoming biological barriers, mesenchymal stem cells (MSCs) have recently become widespread. MSCs exhibit tropism for sites of tissue damage, inflammatory focuses, tumor microenvironment, and have thus gained more attention as vehicles for targeted therapy. One of novel approaches is to create an efficient multifunctional platform using MSCs as a carrier of core-shell polymeric nanoparticles loaded with near-infrared fluorescent dye for dynamic deep-tissue optical monitoring of targeted focuses in mouse body. As a result, the main amount of MSC carrying nanoparticles is accumulated in the inflammatory, cancer and metastasis areas. Hence, a potentially useful MSC-platform that combines their inflammatory/cancer tropism and nanoparticle optical imaging of migration and biodistribution is proposed pursuing MSC-mediated theranostics.

#### Type of presence

Presence online

**Primary author:** Dr GOLOVYNSKA, Iuliia (College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen, China)

**Presenter:** Dr GOLOVYNSKA, Iuliia (College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen, China)

Session Classification: Biomedical Imaging and Nanotechnology

Laser ultrasonics for the excitatio ...

Contribution ID: 19

Type: Invited Talk

## Laser ultrasonics for the excitation of ultrafast acoustics or ultra-intense ultrasounds

Thursday, November 7, 2024 11:00 AM (30 minutes)

In the present talk, I will review the latest results which we have obtained dealing with ultrafast linear and nonlinear acoustics. I will describe our findings related to the excitation of non-destructive shock waves, as well as some results related to the superposition of shock waves for optimum laser excitation.

#### Type of presence

Presence online

Primary author: Dr PEZERIL, Thomas (CNRS)

**Presenter:** Dr PEZERIL, Thomas (CNRS)

Session Classification: Advances in Nonlinear Optics and Laser-Matter Interactions

Proposal for iterative cycles to ob ...

Contribution ID: 20

Type: Invited Talk

# Proposal for iterative cycles to obtain solar cell parameters, in the model of a solar cell diode.

*Tuesday, November 5, 2024 5:10 PM (20 minutes)* 

In this talk, two iterative cycles are proposed to obtain the solar cell parameters: the saturation current, the light current, the series resistance, the parallel resistance and the ideality factor. Obtaining these parameters is of scientific and technological importance, since they provide valuable information for their research, improvement and commercialization.

#### Type of presence

Presence online

Primary author: Dr RANGEL KUOPPA, Victor Tapio (Lancaster University)

Presenter: Dr RANGEL KUOPPA, Victor Tapio (Lancaster University)

Session Classification: Workshop on Sustainable Materials and Technologies

Track Classification: Workshop on Sustainable Materials and Technologies

Type: Poster

# Characterization of novel solar energy converters based on meta-heuristic algorithms

Friday, November 8, 2024 4:48 PM (3 minutes)

The development of photovoltaic technology addresses the challenges posed by the energy crisis. A current priority in this field is to reduce the cost of solar cell (SC) production while achieving properties not typically found in crystalline silicon photovoltaic converters. Consequently, significant attention has shifted toward thin-film, organic, perovskite, and quantum dot solar cells. However, an additional challenge is developing effective methods for characterizing these structures. The SC current-voltage (IV) values are central to their characterization in industry and research. Parameter determination typically involves approximating IV curves using specific models, with metaheuristic algorithms widely employed. Unfortunately, conventional models often cannot be applied to the IV characteristics of the structures above. These challenges necessitate using new models, such as the opposed two-diode model. Furthermore, according to the No Free Lunch theorem, the search for new algorithms capable of effectively solving these novel optimization tasks is crucial. This work compares the effectiveness of 14 metaheuristic algorithms from various classes (evolution-based, swarm intelligence-based, bio-based, chemical & physical-based, humansociety-based, and math-based) for approximating S-shaped IV curves according to the opposed two-diode model. The comparison employed non-parametric statistical methods, specifically the Friedman, Friedman Aligned, and Quade tests. The results demonstrated that the STLBO (Simplified Teaching-Learning Based Optimization) and ADELI (Adaptive Differential Evolution with Lagrange Interpolation Argument) algorithms showed highly competitive performance in accuracy and reliability.

The work was supported by NRFU (project 2023.03/0252).

#### Type of presence

Presence online

Primary author: Prof. OLIKH, Oleg (Taras Shevchenko National University of Kyiv)Presenter: Prof. OLIKH, Oleg (Taras Shevchenko National University of Kyiv)Session Classification: Poster Session

Type: Poster

## Molten salt synthesis of Bi2WO6:Eu

Friday, November 8, 2024 5:01 PM (3 minutes)

Bismuth –containing oxide materials have been attraction much attention as phosphors for light emitting diodes and other devices. Among them these ones containing tungsten are rarely studied due to a low chemical activity of tungsten compounds and high velocity evaporation of WO3 under thermal treatment.

Currently, Bi2WO6 have been attracting significant attention as optical materials/phosphors due to the strong absorption of light by molecular WO4/WO6 anions in the vacuum ultraviolet (VUV) and ultraviolet (UV) spectral regions and further excitation energy transfer to the RE ions and intensive luminescence of the last ones.

Herein, a molten salt approach has been developed to obtain high quality single crystals Bi2WO6 doped with Eu3+ Single crystals have been grown from a high temperature solution containing Na2WO4 as an inert flux. The crystals prepared has been characterized by means of powder X-Ray diffraction, scanning electron microscopy, energy-dispersive X-ray spectroscopy analysis, and infrared spectroscopy (IR).

The peculiarities of luminescence spectra of Bi2WO6 has been studied under UV excitation under room temperature.

#### Type of presence

Presence at Taras Shevchenko National University

Primary author: Mr ORIEKHOV, Stanislav (Taras Shevchenko National University of Kyiv)

**Co-authors:** Dr TEREBILENKO, Kateryna (Taras Shevchenko National University of Kyiv); Dr SLOBODYANIK, Mykola (Taras Shevchenko National University of Kyiv)

**Presenters:** Dr TEREBILENKO, Kateryna (Taras Shevchenko National University of Kyiv); Mr ORIEKHOV, Stanislav (Taras Shevchenko National University of Kyiv)

Session Classification: Poster Session

Type: Oral

### **Bismuth-based Solid State Phosphors: Design, Structural Diversity, and Luminescence Properties**

Friday, November 8, 2024 11:05 AM (15 minutes)

Bismuth -containing phosphors contain multiple tetrahedral anions currently provide novel phosphors generation with improved functionality emerges, posing new challenges and opportunities in material science. The application of monovalent substitution by other rare-earth metals has been the focus of recent intense investigations because of the possible charge transfer processes, which brings the possibility of tailoring the luminescence properties of doped materials, thereby generation highly emissive compounds for useful applications such as light-emitting diods. The effect of dopant concentration, crystal structure, reagents reactivity and reaction medium on the growth of phosphor crystals. Understanding the role of various thermodynamic and kinetic parameters enables the controlled synthesis of complex gadolinium oxides that can exhibit unique tailored properties. Selected application prospects arising from such capabilities are then discussed. One of the advantages of bismuth molybdate and tungstate hosts for RE ions is related with weak concentration quenching of luminescence that related with these ions, particularly Eu3+ ones. Layered crystal structure of mixed-anion compounds studied with general formula A2R(PO4)(MO4), where A = Na or K; R = Y, Bi or RE; M = Mo or W. Although the first structure of this family, Na2Y(PO4)(MoO4), was reported more than three decades ago, there are some gaps in the studies of such compounds from viewpoint of both crystal structure and their physicochemical properties. The further studies of luminescence of K2Bi(PO4)(MoO4):Eu has been shown that its quantum yield is close to 96 % and 86 % when PL excitation performed at 394 and 465 nm, respectively.

#### Type of presence

Presence at Taras Shevchenko National University

Primary author: Dr TEREBILENKO, Kateryna (Taras Shevchenko National University of Kyiv)

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**Presenter:** Dr TEREBILENKO, Kateryna (Taras Shevchenko National University of Kyiv)

Session Classification: Luminescent Materials and Photonic Applications

Type: Invited Talk

## Progress in gallium oxide solar blind UV-C detectors

Tuesday, November 5, 2024 4:30 PM (20 minutes)

Ga2O3 is an ultra-wide bandgap semiconductor that enables the fabrication of solar-blind UV-C radiation detectors without the need for filters to reject visible, UV-A and UV-B daylight. Applications of this type of detector include the monitoring of sanitization processes and hydrogen combustion, along with the early detection of corona effects in power grid lines and high-voltage components.

Ga2O3 can crystallize in several polymorphs, the most common ones being beta and kappa, each with different properties and fields of applications. Beta-Ga2O3, the thermodynamically stable polymorph, is the most investigated for high-power electronic applications although its anisotropy, due to the monoclinic crystallographic phase, poses some problems in the practical realization of devices. The alpha and kappa metastable polymorphs, on the other hand, exhibit a higher symmetry lattice (corundum and orthorhombic respectively), which allows for easier epitaxial growth conditions and processing.

We will present our results regarding the MOVPE growth of Ga2O3 films, their electrical characterization and the fabrication of different kind of UV-C sensor prototypes based on Ga2O3. Beside standard photoresistors and p/n heterojunctions, organic polymers and small molecules were deposited on top of crystalline and amorphous n-type Ga2O3 epilayers, both Si-doped and unintentionally doped, to realize prototypes of solar blind UV-C sensors.

#### Type of presence

Presence online

Primary author: Dr BOSI, Matteo (IMEM CNR)

Presenter: Dr BOSI, Matteo (IMEM CNR)

Session Classification: Workshop on Sustainable Materials and Technologies

Track Classification: Workshop on Sustainable Materials and Technologies

Type: Poster

## Spectroscopic study of ibuprofen interaction with polyethylene glycol matrix

Friday, November 8, 2024 4:15 PM (3 minutes)

Quantum chemical calculations of the structure and IR spectra of ibuprofen molecule were performed using various methods (HF, DFT, MP2). Several different conformers of ibuprofen were considered. The calculation results were compared with the experimentally registered spectra of ibuprofen. It is shown that MP2 method is the most appropriate for the description of the experimentally registered spectrum of ibuprofen.

FTIR spectra of pure ibuprofen and polyethylene glycol (PEG 400) as well as their solutions with different concentrations were registered and analysed. The obtained results of IR spectroscopy of a mixture of polyethylene glycol and ibuprofen (at a concentration of 30%) indicate the potential for controlled release of ibuprofen in pharmaceutical formulations with a polyethylene glycol matrix. This can contribute to the creation of new dosage forms that provide a constant and controlled release of the active substance, which can improve the effectiveness of therapy and the convenience of use for patients.

The work was supported by the National Research Foundation of Ukraine in the frame of the project "Nanostructural modification of application drugs for military medical technologies" (No. 2023.04/0140).

#### Type of presence

Presence online

**Primary author:** RUDENOK, Tetiana (Faculty of Physics, Taras Shevchenko National University of Kyiv)

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Presenter: RUDENOK, Tetiana (Faculty of Physics, Taras Shevchenko National University of Kyiv)

Session Classification: Poster Session

Type: Oral

### Stimulated Raman scattering microscopy: theory and applications

Thursday, November 7, 2024 1:30 PM (30 minutes)

Since its discovery in 1928, Raman spectroscopy has become a powerful tool for molecular identification due to its ability to detect molecular fingerprints. It is widely applied in various fields such as pharmacology, food analysis, and mineralogy. The integration of Raman spectroscopy with optical microscopy has advanced hyper-spectral imaging, enabling detailed spectral acquisition within sample volumes. This breakthrough offers new opportunities in drug industry quality control, biomedical tissue function research, and numerous other fields. However, its broader application is limited by the low Raman scattering cross-section (~10<sup>-30</sup> cm<sup>2</sup>) and interference from fluorescence. Non-linear coherent Raman techniques, such as Coherent Anti-Stokes Raman Scattering (CARS) and Stimulated Raman Scattering (SRS), offer promising solutions. CARS enhances the detectable signal by coherently summing Raman scattered light, reducing image acquisition time by more than 10 000 times compared to spontaneous Raman scattering. This enables the development of fast video-rate Raman microscopy. SRS, which is free from the non-resonant background signal inherent to CARS, produces spectra identical to traditional Raman spectra, simplifying data interpretation and allowing the use of existing molecular fingerprint databases. A further step, Stimulated Raman Gain and Opposite Loss Detection (SRGOLD), addresses limitations in SRS signal detection, enhancing the detected signal and facilitating biomedical applications of the SRS technique.

This progress in Raman-based imaging techniques holds great potential for expanding the practical applications of molecular diagnostics and research.

#### Type of presence

Presence online

Primary author: Dr SHYNKAR, Vasyl (HORIBA Scientific)

Presenter: Dr SHYNKAR, Vasyl (HORIBA Scientific)

Session Classification: Advances in Nonlinear Optics and Laser-Matter Interactions

Type: Oral

### Nonlinear Characteristic of Sinogram for White X-ray and Superiority ART method rather than Fourier transform method for CT-imaging Reconstruction

Friday, November 8, 2024 6:15 AM (10 minutes)

So far, the CT-imaging reconstruction algorithm mainly use Fourier transform method and ART(Algebraic Reconstruction Technique)method. Especially Fourier transform method is based on that the sinogram is linear for X-ray(single color)absorption coefficient on the object materials. However strictly speaking, usual CT use White X-ray, then the sinogram is not linear for X-ray absorption coefficient. For this reason, in low energy region of X-ray photons or in the case of the metal of object, X-ray absorption coefficient is relative large, then the nonlinearity effect of sinogram appears. When the Fourier transform method generates the noise(artifact) of imaging. So I can show that ART method conquers this non-linear problem of sinogram mathematically. This proof is constructed as a following. First this nonlinear sinogram expression divide two parts, one is the related part of X-ray photon energy distribution, one is the part of exponent containing the linear sinogram. Next digitalizing and giving some suitable condition, this sinogram expression become to the fundamental modeling expression of ART method. So ART method conquer. This mathematical proof means that we have established the strong approach by using ART method theoretically. So this consideration will contributed to more developments for Sequential Approximation Method(Gordon, 1970) or SIRT(Simultaneous Iterative Reconstruction Technique) method as the computing realization of ART method.

#### Type of presence

Presence online

**Primary authors:** SUZUKI, Takaharu (Shizuoka University); Prof. AOKI, Toru (Shizuoka University)

Presenter: SUZUKI, Takaharu (Shizuoka University)

Session Classification: Imaging Techniques, CT Imaging, and Augmented Reality

Type: Oral

## Identification of composite material using CT imaging

Friday, November 8, 2024 6:35 AM (10 minutes)

Many of the various products in the world are composed of multiple materials. For example, snacks such as chocolate are sold packed in plastic or paper, and smartphone charging cables have metal power lines covered with nylon. These products can be distinguished by the eyes, but some composite materials cannot.

In X-ray imaging by photon counting using a CT system, X-rays pass through the subject, and directly converted into electrical signals, then projected as an image. Since the energy information of each X-ray is counted during direct conversion, the energy characteristics of the photographed object can be collected. Therefore, it has the advantage of being able to perform material discrimination using that.

In this study, the goal is to identify composite materials that are similar in composition and shape using CT imaging. At first, we imaged a section of the target composite material with a 150kV CT device, reconstructed, and displayed as image data in DICOM format. After adjusting the window width, we were able to capture each of the materials that make up the composite to some extent. Then same imaging was performed in 14 energy bands with thresholds from 10 keV to 150 keV in 10 keV increments, and we compared the reconstructed images.

#### Type of presence

Presence online

Primary author: TAKEMOTO, Shunsuke (Shizuoka Univ.)

**Co-authors:** KASE, Hiroki (Shizuoka University); NISHIZAWA, Junichi; TAKAGI, Katsuyuki; AOKI, Toru (Shizuoka University)

Presenter: TAKEMOTO, Shunsuke (Shizuoka Univ.)

Session Classification: Imaging Techniques, CT Imaging, and Augmented Reality

Type: Oral

### Simulation of Micro-metal Detection with Backscattered X-ray

Friday, November 8, 2024 5:55 AM (10 minutes)

Backscattered X-ray imaging is a nondestructive inspection that uses X-rays scattered backward from an object.

Compared to X-ray transmission imaging, backscattered X-ray imaging has the advantage that the source and detector can be placed on the same side of the object. It is currently used to inspect thick objects and structures.

Although material decomposition methods using X-ray energy information have been proposed, X-ray image and CT images are not effective for small objects such as thin films. Imaging requires a high magnification rate, which imposes strong constraints on the size of the object and the imaging system.

Therefore, we propose a method to detect target micro-metals from materials composed of miscellaneous elements by spectral analysis of backscattered X-rays. In this paper, using the PHITS , particle and heavy ion transport code, the detection of backscattered X-rays from a subject with a PCB(Printed Circuit Board)-like structure using a CdTe detector was simulated. The subject is a layered structure consisting of tin, noble meta, copper, and glass epoxy. Spectra obtained from each of the individual elements, from the complete subject, and from the subject with noble metals excluded were compared and analyzed. The results suggest the possibility of using X-ray fluorescence to detect small objects and a future material decomposition methods in backscattered X-ray imaging.

#### Type of presence

Presence online

Primary author: HAYASHI, Kohei (Shizuoka University)

**Co-authors:** KASE, Hiroki (Shizuoka University); Mr TAKAGI, Katsuyuki (Shizuoka University, ANSeeN Inc.); Prof. AOKI, Toru (Shizuoka University, ANSeeN Inc.)

Presenter: HAYASHI, Kohei (Shizuoka University)

Session Classification: Imaging Techniques, CT Imaging, and Augmented Reality

Type: Poster

## Fluorescence spectra of Ukrainian beers: machine learning exploratory study

Friday, November 8, 2024 5:04 PM (3 minutes)

Beer is one of the most popular drinks in the world. It is produced both at large-scale factories and in small craft breweries. Both producers and distributors of beer require cost-effective and stable ways to control and verify the authenticity of the drink. Traditional methods of evaluating beer properties are often expensive and require significant resources [1]. Recently, the industry has turned its attention to classification using machine learning, which has contributed to the development of rapid, contactless and automated approaches to assess the quality of beer based on spectral data.[2]

The paper examines the potential of a simple 3D printed spectral device in combination with machine learning to classify beers produced by Ukrainian breweries, based on their luminescence spectra. The spectra of 29 samples of Ukrainian mass and craft-produced beers were recorded. ML classification models (KNN, Decision Tree, Random Forest) were applied to classify the samples according to such properties as the scale of the production (industrial vs. craft), storage condition (can vs. bottle), and fermentation type (top vs. bottom). The results of the study indicate that machine learning techniques can be useful for classifying fermented beverages. The models demonstrate relatively high accuracy, although partially limited by the small number of tested samples.

#### **References:**

Gonzaler V.C et al, Journal of the Science of Food and Agriculture , 2018, 98.2, pp. 618-627.
 Gao, Yi-Fang, et al. Food Chemistry, 2024, X 22, pp. 101300

#### Type of presence

Presence at Taras Shevchenko National University

**Primary authors:** YABLOCHKOVA, Kateryna (Taras Shevchenko National University of Kyiv); DANIL-IUK, Dmytro (Taras Shevchenko National University of Kyiv)

Presenter: DANILIUK, Dmytro (Taras Shevchenko National University of Kyiv)

Session Classification: Poster Session

Type: Poster

## The theory of structure formation of electron-hole liquid in dichalcogenides under optical pumping

Friday, November 8, 2024 5:07 PM (3 minutes)

We consider formation of EHL in a transition metal dichalcogenide monolayer in a stochastic approach. The theoretical foundations were formulated in [A.A. Chernyuk et al., Physics Letters A 384, 126185 (2020)] for studying exciton liquid formation in semi-conductor quantum wells. In this work, an exciton gas is created in dichalcogenide plane by pumping. The exciton flux through the island boundary is determined by differ-ence between excitons entering the island and electronhole pairs leaving it. The prob-ability of structure appearance and their configurations is estimated from the distribution function. The kinetic equation for particles number in an island is solved together with the exciton diffusion equation, taking into account the pumping. The interaction between islands occurs through diffusion fields of free excitons.

We obtained that the sizes of EHL islands are tens of microns in monolayers of MoS2 and MoTe2, and the distance between them is hundreds of microns, which is sig-nificantly larger than the corresponding EHL sizes in semiconductor structures with quantum wells.

In case of uniform strip-shaped pumping, the EHL islands are located equidistantly along the strip line, if the strip width is small. If the pumping is performed with a thick strip, then the optimal arrangement of island rows becomes like "checkerboard pattern", and the distance between islands in a row decreases with growing pumping intensity. The number of island rows enlarges with increasing pumping strip thickness.

The arrangement of EHL islands in dichalcogenide layer is an example of macro-scopic lattice in a 2D structure.

#### Type of presence

Presence at Taras Shevchenko National University

Primary author: Dr CHERNYUK, Andriy (Institute for Nuclear Research, NAS of Ukraine)

Presenter: Dr CHERNYUK, Andriy (Institute for Nuclear Research, NAS of Ukraine)

Session Classification: Poster Session

Type: Oral

## Direct laser writing in maskless photolithography technology

Wednesday, November 6, 2024 9:40 AM (20 minutes)

Direct laser writing (DLW) has become a leading technology for creating diffractive optical elements (DOE), particularly for submicron structures. As subwavelength optical devices such as photon sieves and metadevices are developed, the need for precise micro- and nanoscale structures grows. Conventional optical systems, limited by the diffraction limit, struggle to form elements smaller than the optical wavelength. Advanced technologies like electron beam lithography (EBL) and focused ion beam lithography (FIBL) offer higher precision but are costly and slow. A key development in DLW is the implementation of optical systems that exceed the diffraction limit. These systems often use nonlinear recording media with Gaussian beam distribution and special photoresists, enabling resolution enhancement. Saturated absorbers, such as chalcogenide materials, help further improve resolution by spatially reducing beam size. Recent research has explored non-Gaussian beams, like those modeled by a zeroth-order Bessel function, achieving 35-40% size reduction of recorded structures. Picosecond and femtosecond lasers also contribute to higher precision by minimizing thermal diffusion. For submicron DOE production, specialized photoresists like Heat Mode Resists (HMR) and inorganic chalcogenide semiconductors are utilized. They enable submicron exposure and yield structures as small as 130 nm, about one-third the wavelength of the laser. Optimization of DLW relies on adaptive algorithms that adjust laser parameters based on material properties, enhancing the accuracy and uniformity of created elements. These innovations are pushing the limits of DLW, making it a powerful tool for the fabrication of high-performance optical components. The authors express their deep gratitude to the National Research Foundation of Ukraine for financial support under the project No. 2023.04/0004.

#### Type of presence

Presence online

**Primary author:** Prof. PETROV, Viacheslav (Institute for Information Recording of National Academy of Sciences of Ukraine)

**Co-authors:** Prof. KRYUCHYN, Andriy (Institute for Information Recording of National Academy of Sciences of Ukraine); Dr BELIAK, Ievgen (Institute for Information Recording of National Academy of Sciences of Ukraine)

**Presenter:** Dr BELIAK, Ievgen (Institute for Information Recording of National Academy of Sciences of Ukraine)

**Session Classification:** Workshop on Direct Optical Lithography for Advanced Opto- and Microelectronics

Type: Invited Talk

## Science at the FXE instrument of European XFEL

Monday, November 4, 2024 2:00 PM (30 minutes)

The FXE instrument enables ultrafast pump–probe experiments on timescales below 100 femtoseconds, catering to a broad scientific user community. FXE features two independent secondary X-ray emission spectrometers alongside a 1-Mpx detector for scattering studies. Its primary research focuses on the dynamic studies of chemical and biochemical reactions in liquids, as well as various solid-state applications. Utilizing a powerful laser as the pump source, FXE facilitates femtosecond time-resolution studies, leveraging a suite of hard X-ray tools to observe different phenomena.

This presentation provides a basic introduction to the techniques available at FXE, detailing their implementation and the types of information they can reveal about the studied systems. Additionally, we will present examples of recent measurements. Several selected showcase experiments will be discussed to demonstrate how the infrastructure at FXE can be employed to address various scientific challenges.

#### Type of presence

Presence online

Primary author: Dr BIEDNOV, Mykola (European XFEL)

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Presenter: Dr BIEDNOV, Mykola (European XFEL)

**Session Classification:** Exploring Ultrafast Phenomena with the XFEL: Instruments, Capabilities, and Applications

Track Classification: USyNC Workshop

Type: Oral

### X-ray and alpha-ray detection properties of TlBr polycrystalline films

Friday, November 8, 2024 7:45 AM (10 minutes)

Thallium bromide (TlBr) is a semiconductor material with a band gap of 2.68 eV. TlBr has a large atomic number (81, 35) and a high density (7.56 g/cm 3), and therefore exhibits high absorption efficiency for X-rays and gamma rays. Due to these excellent physical properties, TlBr is being researched as a suitable material for semiconductor detectors operating at room temperature. TlBr has a low boiling point and can be easily volatilized by resistance heating in a vacuum atmosphere, making it possible to form a thin film by vacuum deposition. Film formation by vacuum deposition may be suitable for the manufacture of X-ray FPDs (Flat Panel Detectors) that require a large area. A 30um thick film was obtained by vacuum deposition. Measurements by XRD, FE-SEM, and EBSD revealed that the film was a TlBr polycrystalline film with a grain size of 5 - 10  $\mu$ m. When a bias voltage was applied to the TlBr film and X-rays were irradiated, the current increased. 241Am alpha rays were irradiated, a pulse signal was measured. This study demonstrated the possibility of fabricating radiation detectors using TlBr films by vacuum deposition.

#### Type of presence

Presence online

Primary author: TOYOTA, Kouhei (Shizuoka University)

**Co-authors:** KASE, Hiroki (Shizuoka University); NISHIZAWA, Junichi; TAKAGI, Katsuyuki (Shizuoka University, ANSeeN Inc.); AOKI, Toru (Shizuoka University, ANSeeN Inc.)

Presenter: TOYOTA, Kouhei (Shizuoka University)

Session Classification: Radiation Detectors and Detector Materials

Type: Oral

## Design of an optical system with off-axis parabolic mirrors for THz system

Friday, November 8, 2024 12:20 PM (15 minutes)

A terahertz (THz) range of an electromagnetic spectrum is considered to be used for the 6G wireless network. The important task of such networks is to design a collimated beam to increase the working distance between a source and a THz detector. One of the methods for rapid and targeted data transfer is applied directional beamforming technologies using interference of several antennas. Here for such purpose the possibility of off-axis parabolic (OAP) mirrors usage was studied. An optical system with two OAP mirrors for collimation and focusing 140THz radiation on the pyroelectric detector surface is considered.

A Gaussian type of the radiation beam based on experimental data was generated with Ansys Zemax OpticStudio software. As an optical system high-reflectivity OAP mirrors of aluminum with a protective coating with a diameter 50.8mm and reflected focal length 101.6mm were used. For a 140GHz source with a total power of 22mW, Gaussian initial beam profile in the emitter plane and divergence angle of  $22^{\circ}$  at  $1/e^2$  level with peak radiant intensity 0, 3W/sr, collimated beam has been received with divergence angle less than  $3^{\circ}$  and peak radiant intensity 94, 3W/sr.

The divergence angle  $= 2 \times d \ 3^{\circ}$  caused by diffraction was calculated by equation d = /w[rad], where wavelength = 2.14mm corresponds to the 140GHz frequency and w = 25mm is an average mirror semidiameter. The diffraction angle value is comparable to that determined in geometric optics approximation.

This work was supported by the Volkswagen Foundation Partnerships-Cooperation Project 97738.

#### Type of presence

Presence online

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**Presenter:** Mr SHEKERA, Andrii (V.E. Lashkaryov Institute of Semiconductor Physics NAS of Ukraine)

Session Classification: Advanced Optical Systems: From Design to Construction

Type: Oral

## Optimization of Back Surface Field (BSF) Layers for Efficiency Enhancement in CZTS Thin-Film Solar Cells

*Tuesday, November 5, 2024 6:15 PM (15 minutes)* 

Copper Zinc Tin Sulfide (CZTS) thin-film solar cells have gained significant attention as a promising alternative to traditional photovoltaic technologies, owing to their use of earth-abundant, nontoxic materials. A critical factor in enhancing the efficiency of these cells is the incorporation of a Back Surface Field (BSF) layer. The BSF layer plays a key role in minimizing electron recombination at the rear interface, thereby improving charge carrier collection and overall device performance. This abstract reviews the role of the BSF layer in CZTS solar cells, focusing on material selection, fabrication techniques, and optimization strategies. By addressing current challenges and evaluating the impact of BSF integration, this study aims to highlight the potential of BSF-enhanced CZTS cells in making thin-film photovoltaics more efficient and scalable for widespread renewable energy applications.

#### Type of presence

Presence online

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Session Classification: Workshop on Sustainable Materials and Technologies

Type: Oral

## First-principles calculations to investigate the optical properties of ASnO3 (A = Ba, Ca, Sr, and Mg) perovskite oxides for the optoelectronic applications

*Tuesday, November 5, 2024 11:55 AM (15 minutes)* 

Advances in material engineering have demonstrated the high stability and low toxicity of tinbased perovskites, presenting an excellent lead-free alternative. Consequently, an ab initio study was conducted to investigate the structural, electronic, and optical properties of the tin-based perovskite oxides ASnO3 (A = Ba, Ca, Sr, Mg). The structural parameters showed highly consistent results with previous experimental and theoretical findings. The electronic calculations revealed semiconductor characteristics with indirect bandgaps. Analysis of the optical properties indicated significant absorption behaviour and weak reflection performance. Overall, these tin-based perovskite oxides hold great potential as materials for the electronic industry, particularly in optoelectronic applications.

#### Type of presence

Presence online

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Session Classification: Workshop on Sustainable Materials and Technologies

Type: Poster

## Optimization of CdxTeyOz Nanocomposite Film Synthesis via the SILAR Method for Controlled Structural and Phase Properties

Friday, November 8, 2024 5:10 PM (3 minutes)

This study focuses on the synthesis of CdxTeyOz films using the SILAR (Successive Ionic Layer Adsorption and Reaction) method, a cost-effective chemical deposition technique that enables precise control of nanocomposite structures. By investigating two batches of films with varying treatment cycles (five and ten), the research highlights the relationship between synthesis conditions and the resulting structural and phase properties. The first batch, with fewer cycles, yielded thinner films with a more uniform structure, while the second batch exhibited increased layer thickness and material accumulation, leading to a more irregular surface morphology.

The study employed advanced characterization techniques such as scanning electron microscopy (SEM), X-ray diffraction (XRD), and energy-dispersive X-ray spectroscopy (EDX). These methods confirmed the formation of a CdxTeyOz nanocomposite layer on a CdS/ZnO substrate, with differences in the chemical composition and crystallinity between the two batches. The experimental findings suggest that the SILAR method allows for fine-tuning the properties of the resulting nanocomposite films, which can have potential applications in photovoltaics, photocatalysis, and sensor development.

Overall, the research contributes to optimizing the SILAR process for producing nanocomposites with targeted electronic and optical properties. Future work will focus on further refining the synthesis parameters to enhance material homogeneity while maintaining the advantages of the SILAR method in terms of cost-effectiveness and structural control.

#### Type of presence

Presence at Taras Shevchenko National University

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Type: Oral

## Human stem cells carrying polymer nanoparticles with visible and near-infrared dyes for dynamic imaging of inflammatory focuses in the brain

Friday, November 8, 2024 2:35 PM (10 minutes)

The chronic inflammation in the brain is one of the main causes of neuronal cell death and the progression of neurodegenerative disease. Currently, nanoparticles (NPs) are widely used because they have unique properties that make them suitable for diagnostics and treatment. However, NPs face different biological barriers that limit their successful biodistribution. The blood-brain barrier (BBB) is a main and highly selective semipermeable border of endothelial cells that regulates the transfer of solutes and chemicals between the circulatory system and the central nervous system. To solve the problem of overcoming BBB, mesenchymal stem cells (MSCs) have recently become widespread. MSCs have a certain innate homing ability toward the site of inflammation and have thus gained more attention as vehicles for targeted neuroinflammation therapy. The objective of the study was to create a novel, active, and multifunctional platform using human MSCs as a carrier of core-shell polymeric nanoparticles (NPs) loaded with fluorescent dye in near-infrared (NIR) or visible range for dynamic monitoring of lipopolysaccharides (LPS)-induced inflammatory focus in the mouse brain. As a result, the main amount of MSC carried with NPs, is accumulated in the inflammatory focus of the brain. Hence, a potentially useful MSC platform that combines their inflammatory tropism and multimodality NP optical imaging of migration and distribution is proposed for pursuing MSC-mediated theranostics against brain inflammation.

#### Type of presence

Presence online

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Presenter: BARI, Rana Zaki Abdul

Session Classification: Biomedical Imaging and Nanotechnology

Type: Oral

## Engineering of Plasmonic Anisotropic Nanopatch-Based Metasurfaces

Thursday, November 7, 2024 4:15 PM (15 minutes)

Hyperbolic metasurfaces are known for their dispersion and polarization properties, such as negative refraction, hyperlensing, enhanced spontaneous emission, etc [1]. The surface waves localized at hyperbolic metasurfaces are called hyperbolic plasmon-polaritons and exhibit a lot of potential applications for planar technologies [2].

In this work, we analyze the dependencies of the spectral positions of the resonances and spectral bandwidth of hyperbolic regime for the metasurfaces based on square arrays of the nanodisks [3] and rectangular nanopatches. Namely, we study the resonant characteristics of metasurfaces by varying the size of the nanoparticles, the degree of stretching (anisotropy) and the period of the metasurface from the isotropic to extreme anisotropic cases. As a result, we defined the quadratic dependence of the spectral bandwidth for one of the resonances on the anisotropy degree, when the electric field is oriented along the stretching direction. Besides, we demonstrate the plasmon canalization, which is characterized by a flat isofrequency contour and the self-collimated unidirectional propagation of surface wave. The canalization takes place in the vicinity of one of the resonances highlighting the relevance of the metasurface engineering for the in-plane optical signal transferring.

A.H. acknowledges the support from IEEE Microwave Theory and Technology Society (IEEE MTT-S) within the Undergraduate/Pre-Graduate Scholarship.

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#### Type of presence

Presence online

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Session Classification: Advances in Metasurfaces and Plasmonic Nanostructures

Type: Oral

## Dependence of the random lasing threshold and spectrum of dyes on the parameters of the active scattering medium

Thursday, November 7, 2024 2:00 PM (15 minutes)

In multiply scattering media, there is the possibility of light lasing without optical resonator. This phenomenon is possible due to the formation of positive feedback resulting from the repeated extension of the path of a scattered photon in the active region and called random lasing.

The main parameters that influence the occurrence of random lasing in the active medium are: the concentration of scattering centers, dye concentration, and temperature. Vesicular films provide the most efficient light scattering. The concentration of vesicles in the films determines the degree of elastic light scattering in the sample. As the concentration of vesicles increases, the efficiency of elastic scattering in the active medium increases.

Increasing the concentration of dye molecules in the film increases the probability of photon interaction with these molecules. Lowering the temperature affects the process of random lasing by reducing the threshold intensity for its occurrence. Low temperature promotes more efficient amplification in the active medium due to reduced reabsorption of random lasing radiation caused by the overlap of the amplification spectral contour with the absorption band.

Based on experimental data, it has been shown that increasing the concentration of vesicles and dye molecules, and a lowering the temperature, leads to a reduction in the random lasing threshold. Increasing the concentration of vesicles and dye molecules, along with lowering the temperature, leads to a broadening of the random lasing spectrum and its shift toward the long-wavelength region. A decrease in temperature results in a broadening of the random lasing spectrum and to shift to short-wavelength region.

Keywords: random lasing, laser dyes, strongly scattering media, vesicular polymer films.

#### Type of presence

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Session Classification: Advances in Nonlinear Optics and Laser-Matter Interactions

Type: Poster

## Dynamical Diffraction Model for Analyzer-Based Imaging

Friday, November 8, 2024 4:18 PM (3 minutes)

The analyzer-based imaging (ABI) is one of the most sensitive phase-contrast methods for weakly absorbing objects with low background due to high angular selectivity of analyzer crystal to scattered radiation. The most of the common approaches of ABI modelling are based on the approximation of geometrical optics for scattering in the non-crystalline sample and even in the analyzer crystal. At the same time, more rigorous theories for describing the radiation diffraction in the analyzer crystal, for example, based on the use of point spread functions are applied. However, these theories often use the formulas based on approximation, which valid only for smooth displacement fields and, therefore, cannot be quantitatively correct for describing the X-ray diffraction on the analyzer crystal with microdefects.

We propose another approach for theoretical description of ABI images that is based on a rigorous theory of multiple (dynamical) scattering in the non-crystalline sample, as well as in the monochromator and analyzer crystals. The corresponding theoretical model allows taking into account complete multiplicity of X-ray scattering in the single crystals, as well as in the non-crystalline sample. Calculated profiles of intensity, obtained in terms of the proposed theoretical model, are in a good agreement with the previously published calculated results and experimental data for the model objects. In addition, suggested approach allows taking into account structure imperfections in crystals of both the monochromator and the analyzer, which can cause great influence on the reflection curve and consequently on the resulting image.

#### Type of presence

Presence at Taras Shevchenko National University

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Type: Oral

## Realistic Photon-Number Resolution and Its Impact on Gaussian Boson Sampling

Friday, November 8, 2024 8:50 AM (15 minutes)

Gaussian boson sampling (GBS) (see Ref. [1]) is a promising quantum computing model that exploits photonic systems to perform computations beyond the reach of classical methods. A crucial aspect of GBS is the detection of photon patterns at the output of an interferometer. However, most experiments rely on on-off detectors that can only identify whether photons are present, without resolving the exact number of photons. While photon-number resolving (PNR) detectors offer the ability to accurately count photons, building perfect PNR detectors remains a challenge due to technical limitations.

In this talk, we present a theoretical framework that models GBS experiments using realistic photon number resolving detectors, see Ref.[2]. We derive a probability distribution for photoncounting that accounts for detector imperfections and can be adapted for both on-off and imperfect PNR detectors. This distribution is expressed in terms of matrix functionals, such as the Hafnian and Torontonian, which are central to the description of different types of photodetectors.

By implementing realistic photon number resolution in our model, we explore how detection imperfections affect the overall performance of GBS experiments. We also propose validation techniques that are robust to these imperfections. This work contributes to the improvement of experimental setups and paves the way for more accurate GBS-based quantum technologies, with potential applications to computational problems that are hard to solve on classical computers.

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#### Type of presence

Presence at Taras Shevchenko National University

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Session Classification: Quantum Optics and Photonic Information Processing

Type: Poster

## Structural and spectroscopic insights into Sodium-Europium(III) orthophosphate

Friday, November 8, 2024 4:55 PM (3 minutes)

Recently, increasing attention has been tuned to luminescence behaviour related to structure specialty of phosphor materials because microstructure of host material decides the fluorescence properties [1]. Phosphate is a good type of candidate for its reasonably large band gap, high thermal and chemical stability. The basic building block of phosphates is the PO4 tetrahedron and EuOx, which is flexible and can inhabit various coordination environments by altering the Eu–O bond lengths in the wide range of 2.55⊠3.13 Å [2]. Moreover, combining EuOx octahedra with PO4 tetrahedra may construct various structures in which these polyhedra are interconnected via common O atoms.

Although the spectroscopy of K3Eu(PO4)2 has been currently well studied, replacing the cation with sodium can have a positive effect on the properties of the obtained Na3Eu(PO4)2. Based on single crystal data, the structure consists of PO4 tetrahedra and isolated europium polyhedra, which together form the structural type of glaserite.

The synthesis of Na3Eu(PO4)2 has been carried out by single crystal growth technique and by the solid-state method. The peculiarities of Na3Eu(PO4)2 as a perspective phosphor has been discussed taking into consideration IR, luminescence spectroscopy and X-ray single crystal diffraction analysis.

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- Ju, G., Hu, Y., Chen, L., Wang, X., Mu, Z., Wu, H., & Kang, F. (2012). A reddish orangeemitting stoichiometric phosphor K3Eu (PO4) 2 for white light-emitting diodes. Optics & Laser Technology, 44(1), 39-42.

#### Type of presence

Presence at Taras Shevchenko National University

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Presenter: Mrs NESMIIAN, Kateryna (Taras Shevchenko National University of Kyiv)

Type: Poster

### Effect of MoO3 Content on Structural, Thermal and Luminescent Properties of Potassium Phosphomolybdate Glasses

Friday, November 8, 2024 4:21 PM (3 minutes)

Optical properties of various transition-metal ions doped glasses have been under investigation in recent years in view of their technological applications, especially in lasers, phosphors, solar energy converters, plasma display panels and in a number of electronic devices. Molybdenumcontaining glasses possess a variety of specific features, which arouse interest in view of their applications. It is known that the addition of MoO3 enhances the semi-conducting properties of the host glass because of the different valence states of molybdenum. Moreover, there are some data on different coordination environment of molybdenum within a vitreous host. The ratio of different oxygen coordination numbers of molybdenum and the polarizability of the oxygen surrounding the paramagnetic ions depends on the presence of bridging and non-bridging oxygens and on the change of the coordination number.

On the other hand, the MoO3 and Bi2O3 oxides appeared as non-conventional network formers because of the participation of MoO4, MoO6 and BiO6 groups in the formation of the glass network. The bismuth phosphate-based glasses have very wide applications for optoelectronic materials such as laser host fibers for communications and photonic switches.

Herein, the series of glasses P2O5-MoO3-Bi2O3-K2O has been obtained by conventional melt approach. The influence of MoO3 content in a range of 5,0 -30,0 % mol has been studied in a light of structural and spectroscopic properties. Moreover, Eu(III) doping has been used as a structural probe for additional luminescent estimation of coordination environment of Mo within the glassy network.

#### Type of presence

Presence at Taras Shevchenko National University

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Presenter: Mr VOINALOVYCH, Artem (Taras Shevchenko National University of Kyiv)

Type: Poster

## Modification of Borophosphate Glass Composition for Joint Thermal Processing with Molybdenum Oxide for Development of Solar Cell Coatings

Friday, November 8, 2024 4:12 PM (3 minutes)

Glasses based on borophosphate with the formula (45-0.5x)P2O5-xB2O3-10,0MoO3-(45-0.5x)Na2O where  $\boxtimes$  = 20,0-60,0 have been manufactured using the melt-quenching methodology. Molybdenum oxide alone does not rank among glass-forming oxides, but it is able to enter the glass structure in the form of MoO4 tetrahedra or MoO6 octahedra with some glass-forming oxides, like P2O5. The regularities of phosphate-borate glasses modified with molybdenum(VI) oxide with the following composition: (45-0.5x)P2O5-xB2O3 -10.0MoO3 -(45-0.5x)Na2O (x = 20.0-60.0) have been carried out and it is shown that an increase in B2O3 concentration from 45 to 60% mol. is accompanied by an increase in the hygroscopicity of the obtained amorphous materials. To modify the optical properties of the glass, 10% mol of MoO3 has been added to its composition, because with a higher content of this modifier, oxidation-reduction processes Mo(VI) $\rightarrow$  Mo(V) with loss of transparency of the resulting glass is expected.

In order to design luminescent coatings that effectively absorb in the UV region of the spectrum, an activator of 0.1% mol Eu2O3 was introduced into the composition of glasses (45-0.5x)P2O5-xB2O3 -10.0MoO3 -(45-0.5x)Na2O where x = 20-40. As a result of the study, it was found that under the condition of exposure of melts of the composition (44.95-0.5x)P2O5-xB2O3 -10.0MoO3 -(44.95-0.5x)Na2O - 0.1Eu2O3 (x = 20.0-60.0) solubility of europium oxide decreases with increasing B2O3 content.

The glassws has been characterized by IR and luminescence spectroscopy, diffuse reflectance spectroscopy and X-ray powder analysis. It is shown that glass 34.95P2O5 –20.0B2O3 -10.00MoO3 –34.95Na2O –0.1Eu2O3, which is effectively excited by UV radiation, is the most promising for modeling UV to visible light convertors.

#### Type of presence

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Presenter: Mrs SAIENKO, Liliia (Taras Shevchenko National University of Kyiv)

Type: Poster

## **Multilayer coatings for Synchrotron Radiation**

*Monday, November 4, 2024 11:50 AM (10 minutes)* 

V.V. Kondratenko, E.N. Zubarev, Y.P. Pershyn\*, I.A. Kopylets+, A.Yu. Devizenko, L.E. Konotopsky, V.A. Sevryukova, V.S. Chumak

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Our group has experience in the fabrication and study of multilayer coatings, which are mainly used in X-ray optics as multilayer X-ray mirrors (MXMs). These are conventional MXMs based on Be, B, C, Mg, Si, Sc and Ti, as well as heat- and radiation-resistant MXMs, for example: Si/Mg2Si, Mo2B5/B4C, MoSi2/Si, WC/Si, CrB2/C, etc. We have fabricated mirrors, monochromators, collimators, polarizers, objectives, diffraction gratings, supermirrors etc. We have studied thermal and radiation stability of MXMs; the early stage of reaction between layers at sub-nanometer level; and evaluated the thickness, composition and density of reaction products. Some recent results on the application of fabricated multilayer materials in three areas will be presented.

These include: (1) multilayers (MLs) for radiation-resistant materials in nuclear and fusion power applications (using W/quasicrystal multilayers as an example); (2) reflective X-ray masks using WC/Si multilayers; and (3) high-resolution multilayer X-ray mirrors using W/B4C and W/Si material pairs.

#### Type of presence

Presence online

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**Session Classification:** Unifying Efforts: Developing the Ukrainian Synchrotron Community and Research Infrastructure

Track Classification: USyNC Workshop

Type: Poster

#### Fractal Resonators for Use in a Microwave Kinetic Inductance Detector

Friday, November 8, 2024 4:24 PM (3 minutes)

Microwave Kinetic Inductance Detectors (MKID) are widely used for detecting low-energy photons due to their high sensitivity and ease of multiplexing, with applications in astronomy and spectroscopy. This work investigates using Hilbert fractal planar resonators as a substitute for conventional straight or meander resonators in MKID. The study addresses challenges in miniaturizing resonators to increase pixel density. Numerical simulations reveal how MKID sensitivity depends on the substrate thickness, microstrip fractal line width, and density. The results demonstrate significant potential for miniaturizing fractal resonators compared to meander ones due to a more uniform microwave field distribution. A novel method for continuously detecting resonant frequency shifts across multiple resonators simultaneously is proposed, replacing the sequential scanning typically used in MKID. This method, based on processing a multi-tone microwave signal, enables rapid detection without the "dead time" when detector pixels are inactive.

#### Type of presence

Presence online

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Presenter: Dr KALENYUK, O.A. (G. V. Kurdyumov IMP of the N.A.S.U.)

Type: Invited Talk

## Revealing hidden photons: imperfect photocounting measurements and their applications

Friday, November 8, 2024 8:05 AM (30 minutes)

In quantum optics it is widely believed that all measurements with coherent states of light and their statistical mixtures can be explained without the need to quantize the electromagnetic field. Quantum states that do not satisfy this condition are considered to be nonclassical. Nowadays, optical nonclassicality is often considered as an important resource for creating quantum entanglement with linear passive optical elements, quantum computation, quantum metrology, etc.

In real-world scenarios, measurements are imperfect. For example, many photocounting techniques are unable to distinguish between adjacent numbers of photons. These imperfections can dramatically change our conclusions about the quantum nature of light: even experiments with highly nonclassical light can be explained in terms of classical electrodynamics.

In this talk, I will briefly review our recent works related to the theory of realistic photodetection [1-3], noisy free-space channels [4], and highly effective methods for testing nonclassicality under such unfriendly conditions [5,6]. I will discuss whether the impossibility of detecting nonclassicality means it is lost as a quantum resource [7]. Finally, I will present an application of our theory to some models of nonuniversal quantum computation [8,9].

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[3] E. V. Stolyarov, et al., PRA 108, 063710 (2023).

[4] M. Klen, et al., PRA 109, 033712 (2024).

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[6] V. S. Kovtoniuk, et al., PRA 109, 053710 (2024).

[7] V. S. Kovtoniuk, et al., arXiv:2408.04740 [quant-ph] (2024).

[8] V. Ye. Len, et al., Phys. Scr. 97, 105102 (2022).

[9] I. S. Yeremenko, et. al., PRA 110, 043715 (2024).

#### Type of presence

Presence at Taras Shevchenko National University

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Session Classification: Quantum Optics and Photonic Information Processing

Type: Invited Talk

## Electrical characteristics of Cu-electrode CdTe detectors

Friday, November 8, 2024 6:55 AM (20 minutes)

Cadmium Telluride (CdTe) is one of the excellent semiconductor detector materials. However, the long-term stability of the electrode on CdTe has been relatively understudied. CdTe detectors with Cu-electrode were fabricated to analyze stabilities of the junction between the electrode and the crystal. The fabricated detectors demonstrated excellent rectifying properties after electrical aging, indicating low electrical stability. In addition, the long-term electrical characteristics were found to be unstable, as their properties change with storage. The direction of these changes was not consistent, suggesting that the chemical bond between the oxide and Cu electrode and the ratio of the two types of copper oxides could evolve. These results suggest that other metals, including conventional electrode materials, may experience changes in the electrode state over time if they are not completely free of a native oxide layer.

#### Type of presence

Presence online

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Presenter: TAKAGI, Katsuyuki (Shizuoka University, ANSeeN Inc.)

Type: Oral

#### Characterization of Mesa Structure of GaN-based Radiation Detectors

Friday, November 8, 2024 7:15 AM (10 minutes)

Semiconductor radiation detectors with high energy sensitivity are primarily being developed, but there is a demand for semiconductor detectors that can handle low energy levels of around 30 keV or less. Therefore, we propose gallium nitride (GaN) as a new semiconductor detector material, aiming for detectors useful in the low energy range of approximately 10 to 26 keV. GaN has a large bandgap, which reduces thermal noise and allows for operation at room temperature. Additionally, research on GaN for applications in LEDs and power devices has progressed, and its excellent charge transport properties have been demonstrated. Due to these characteristics, GaN is expected to be useful in low-energy applications such as mammography. Up to now, we have prototyped and evaluated both vertical pn-type GaN detectors and pin-type GaN detectors. Based on the results, we have decided to focus on pin-type detectors, which have a high-quality crystal in the active layer, as the basic design. In the future, we plan to further reduce the dark current and increase the thickness of the i-layer. In this study, we fabricated a pin-type detector with a mesa structure, which can apply higher voltage and reduce dark current, along with passivation treatment. The prototype detector exhibited diode characteristics. Additionally, we detected alpha particle pulses, suggesting the potential for future photon counting.

#### Type of presence

Presence online

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**Presenter:** Mr INABA, Kagemitsu (Graduate School of Integrated Science and Technology, Shizuoka University)

Type: Oral

## Electron Beam Doping with CdTe for Radiation Detectors.

Friday, November 8, 2024 7:25 AM (10 minutes)

CdTe as a semiconductor has advantages when used as a radiation detector, such as sensitivity to high energy and the ability to operate at room temperature. However, the disadvantage is that the charge collection efficiency is lower than that of Si and Ge, and a high voltage must be applied to collect a sufficient amount of charge. Therefore, it is necessary to suppress the leakage current associated with the application of high voltages.

To conduct the experiments, we used 0.75 mm thick, 3 mm square Acrorad CdTe crystals and deposited In on one side and Au on the other side to fabricate a sample with an In/CdTe/Au structure. The In side of the sample was doped with an electron beam, which allows local heating and diffusion near the surface. Hall effect measurements revealed an n+ layer doped with In, forming a pn-junction diode with p-type bulk CdTe:Cl. This allows doping of CdTe:Cl, which is thermally sensitive. The sample was evaluated for I-V characteristics and  $\gamma$  spectral characteristics.

As a result of these evaluations, diode-like characteristics were confirmed, and a peak was also confirmed in the  $\gamma$  spectral characteristics.

#### Type of presence

Presence online

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Presenter: SHINMURA, Yuki (Shizuoka University)

Type: Oral

### Development of Compact Neutral Source using D-D Reaction

Friday, November 8, 2024 7:35 AM (10 minutes)

In X-ray imaging, light elements are transmitted through light elements and scattered and absorbed by high-density metals, so the transmitted image shows the metal portions well. In contrast, neutron imaging transmits light elements such as hydrogen through metal and is scattered and absorbed by light elements such as hydrogen, so that the transmitted image shows the areas containing light elements. Thus, x-rays and neutrons have complementary characteristics. However, the practical application of neutron imaging systems is difficult because they require the use of a large accelerator or nuclear reactor as a neutron source, which is a large-scale facility. Therefore, the objective of this study is to realize a compact neutron source for practical use of neutron imaging devices. In this study, a vacuum chamber with a diameter of 0.20 m and a cathode with a diameter of 0.04 m were used. As a neutron generation method, we used the DD reaction, which is expected to be a small-scale facility, because it can cause fusion at lower energy than using an accelerator and because deuterium is a non-radioactive material. Deuterium gas flows into the vacuum chamber, and by applying electric power, the deuterium ions generated are accelerated by the electrodes and collide at the center of the cathode, causing the DD reaction and producing neutrons. The neutron dose rate was then measured at different vacuum levels in the chamber. The actual results were 0.04  $\mu$ Sv/h at 0.1 Torr and 0.08  $\mu$ Sv/h at 0.06 Torr.

#### Type of presence

Presence online

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Presenter: NAKIYAMA, Keigo (Shizuoka Univ.)

Type: Invited Talk

## **Spatial Representation of 3D X-ray CT using Mixed Reality that Matches the Practitioner's Perspective**

Friday, November 8, 2024 5:35 AM (20 minutes)

In recent years, research utilizing Mixed Reality (MR) has garnered attention in medical fields, particularly in radiology. By rendering data acquired from X-ray CT and MRA in 3D and aligning it with the real-world environment, MR can be applied to support diagnostics, simulate surgeries, and assist in medical procedures. However, conventional multi-planar reconstruction (MPR) images of sagittal, axial, and coronal views express 3D voxel information as 2D-pixel data, which differs from the practitioner's view when observing the patient. This makes it difficult to spatially grasp the internal anatomy of the patient. This study aims to use MR to represent the patient's internal structures in 3D and display MPR images aligned with the practitioner's perspective when observing the patient. Systems that employ a head-mounted display (HMD), spatial reconstruction display, and motion capture were proposed. By using the bed position as a reference point, the angle from which the practitioner views the patient was calculated, and MPR images from DICOM data were generated and superimposed on the real-world environment. As a result, practitioners can observe the internal structures of the patient according to their own viewpoint

#### Type of presence

Presence online

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Presenter: Dr KASE, Hiroki (Shizuoka University)

Session Classification: Imaging Techniques, CT Imaging, and Augmented Reality

Type: Invited Talk

### Reciprocal Asymmetric Transmission: A Way Passed From Plane Waves To Metaholograms

Thursday, November 7, 2024 3:15 PM (30 minutes)

Reciprocal Asymmetric Transmission (RAT) has attracted attention of the metamaterial, photonic crystal, and artificial chirality communities since 2000's. Initially, RAT has been understood as the difference in transmission when the structure with broken spatial inversion symmetry is illuminated by the same linearly or circularly polarized wave in forward and backward (i.e., opposite) directions. The diffraction gratings with one-side corrugations are probably the simplest structures enabling RAT. However, they are not well suitable for the achievement of a high-contrast RAT, because it is rather accidental therein. To ensure that zero (i.e., symmetric) order is suppressed, while the desired higher orders are excited only for one direction, photonic-crystal gratings, metamaterial gratings, and gratings involving epsilon-near-zero materials have been proposed. In these structures, dispersion and diffraction work jointly to block zero-order transmission and enable conversion of the incident-wave energy to the selected diffraction orders. Instead of diffractions, polarization states can be used, so that symmetric co-polarized transmission can be suppressed, while asymmetry occurs due to the forward-to-backward contrast in cross-polarized transmission. Metagratings with subwavelength slits, which support surface plasmons, have been the first structures, in which asymmetric field distribution has been demonstrated at beam-type illumination. The recently proposed Janus metasurfaces offer prospective RAT devices, which are used either for generation of asymmetric metaholograms at the identical forward and backward illuminations, or for asymmetric transformation of one hologram to another. To summarize, RAT has a floating focus, being presently shifted towards asymmetric functionality, and expectedly to the general asymmetric physics at the next step.

#### Type of presence

Presence online

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Session Classification: Advances in Metasurfaces and Plasmonic Nanostructures

Type: Oral

## 3D representation for simulation of the feeding situation and feeding of "scalpels and other instruments that approach the body"into the body.

Friday, November 8, 2024 6:25 AM (10 minutes)

In recent years, radiotherapy using diagnostic imaging devices has been used in the medical field. In the treatment of scalpels and other instruments that approach the body, it is now possible to compare CT images for treatment planning and immediately prior to treatment to pinpoint the scalpel insertion. This enables more accurate alignment than the previously possible adjustments made by eye.

However, there are some problems. The human body is highly likely to deviate from the CT image taken immediately prior to treatment, and fine adjustments must be made while the scalpel is being inserted. Detailed adjustments are often based on long years of experience and knowledge, and it takes time to transfer the technique, resulting in a decrease in the number of treatment providers. In order to increase the number of therapists, there is a need for a system to assist therapists that does not depend on knowledge or experience.

The objective of this research is to represent the X-ray CT layer in a 3D representation using MR, and to clearly show in real time where an instrument, such as a scalpel, is located inside a person's body when it is inserted into the body. In this paper, we represent a material such as a sphere created in a Unity 3D project on a spatial reproduction display, and color only the area where a hand or a stick is in contact with it and its surroundings using Unity's shader function, so that the contact area could be determined.

#### Type of presence

Presence online

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Presenter: Mr HORIUCHI, TAKAYA (Shizuoka University)

Session Classification: Imaging Techniques, CT Imaging, and Augmented Reality

Type: Poster

### The Role of GeO2 in the Glass-Ceramic Formation and Microstructure of Sodium Phosphate-Molybdate Glasses

Friday, November 8, 2024 5:13 PM (3 minutes)

Homogeneous glasses and class-ceramics can be produced by molten glass and converting it into a fine-grained ceramic by an appropriate heat treatment. Generally, wide range of glass-ceramic properties can be modified in a predictable way by changing the composition with a suitable heat treatment. The final crystalline phases depend on the composition of the glass and the heating methods. Thus, the properties of glass-ceramics are determined by the heating and annealing procedure during synthesis of glasses and their microstructures, which depend on the composition of the parent glass as well as the thermal treatment.

The peculiarities of the glasses formation based on the P2O5–MoO3–GeO2–Na2O system have been investigated for GeO2 content from 5 to 30 % mol of GeO2 and from 5 to 30 % mol MoO3. The base glass composition has been modified by partial replacement of P2O5 for GeO2. The effect of the compositional variation on the glassy areas and crystallization products of the glasses and the type of the solid solution phases formed as well as the resulting microstructure have been traced by differential thermal analysis (DTA), powder X-ray diffraction analysis (XRD) and scanning electron microscopy(SEM).

The objective of the present work is to understand the role of the glass oxide constituents in determining the type of the crystalline phases formed, their solid solution formed and the microstructure of the resultant glass-ceramic materials.

#### Type of presence

Presence at Taras Shevchenko National University

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Presenter: Mr PASHYNSKYI, Yehor (Taras Shevchenko National University of Kyiv)

Type: Poster

## Tetragonal scheelite structure and bright luminescence of NaBi(MoO4)2 doped with europium(III) Single Crystals

Friday, November 8, 2024 4:03 PM (3 minutes)

Materials based on double molybdates have a promising application in the field of optoelectronic devices[1] due to their physical and chemical properties, and they also exhibit the phenomenon of upconversion, which is widely used in diagnostics, therapy, sensors, solar cells, photocalysis, bio-imaging[2].

The main goal is to obtain pure NaBi(MoO4)2 and NaBi0.5Eu0.5(MoO4)2 with tetragonal scheelite structure, without impurities of molybdenum (VI) oxide. The presence of this type of impurity makes it impossible to accurately determine the physical and chemical properties of compounds of this type, such as luminescence, conductivity, etc.

In this work, we obtained pure compounds NaBi(MoO4)2 and NaBi0.5Eu0.5(MoO4)2 and confirmed their tetragonal scheelite structure and the absence of impurities using the X-ray method, as well as infrared spectroscopy.

[1] Guler, I., Isik, M., & Gasanly, N. (2024). Growth and optical properties of (Na0. 5Bi0. 5)(Mo1- x Wx)O4 (x= 0.25) single crystal: a potential candidate for optoelectronic devices. Optical and Quantum Electronics, 56(1), 17.

[2] Kunchala, R. K., Kalia, R., & Naidu, B. S. (2020). Upconversion luminescence properties of NaBi (MoO4)2: Ln3+, Yb3+ (Ln= Er, Ho) nanomaterials synthesized at room temperature. Ceramics International, 46(11), 18614-18622.

#### Type of presence

Presence at Taras Shevchenko National University

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Type: Oral

## CVD Synthesis of 2D-MoS<sub>2</sub> for Heterostructure Development in Optoelectronic Devices

*Tuesday, November 5, 2024 2:15 PM (15 minutes)* 

Molybdenum disulfide ( $MoS_2$ ), a two-dimensional transition metal dichalcogenide with a direct bandgap in its monolayer form, presents significant potential for a wide range of applications in optoelectronics. The heterostructure formed by combining  $MoS_2$  with gallium nitride (GaN), a wide-bandgap semiconductor characterized by high electron mobility, thermal stability, and favorable optical properties, offers a platform for the development of advanced electronic device architectures.

This work details the synthesis of high-quality  $MoS_2$  monolayers via Chemical Vapor Deposition (CVD) utilizing liquid precursors. The proposed method enables the formation of uniform, largearea  $MoS_2$  flakes with precise control over thickness, morphology, and crystallinity, presenting a scalable approach for the integration of 2D materials. In addition, a process for transferring  $MoS_2$ grown on  $SiO_2/Si$  to GaN substrates is introduced and compared with the direct growth of  $MoS_2$ on GaN.

Furthermore, we present preliminary exploratory results on the integration of  $MoS_2$  into photonic structures, specifically bullseye cavities, to enhance light-matter interaction via the Purcell effect. This integration highlights the potential of  $MoS_2$  for photonic devices, where its unique optical properties can be leveraged to achieve enhanced control over light emission.

The future outcomes of this study aim to demonstrate the versatility of CVD-grown  $MoS_2$  for high-performance optoelectronic applications.

This research was supported, in part, by the PRIN Project "2DIntegrate" (Prot. 2022RHRZN2) funded by MUR under the European Union –Next Generation EU programme.

#### Type of presence

Presence online

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Presenter: Ms ESPOSITO, Fiorenza (CNR-IMEM)

Session Classification: Workshop on Sustainable Materials and Technologies

Track Classification: Workshop on Sustainable Materials and Technologies

Type: Oral

## Applying Deep Learning Approaches to Estimate the Number of Layers in Nanomaterials from Optical Images

*Friday, November 8, 2024 12:35 PM (15 minutes)* 

Atomic-level engineering enables the creation of hybrid structures that enhance light-matter interactions and advance next-generation optical devices. Two-dimensional (2D) materials are important in nanophotonics due to their unique properties.

In this study, the authors introduce a hybrid vision transformer model, termed 2D-HVT, specifically designed for identifying and analyzing 2D materials. This model incorporates the FastViT encoder alongside a composite decoder that merges LRASPP and Knet, optimizing inference speed without compromising accuracy in assessing the thickness of molybdenum disulfide (MoS2) layers, which may range from monolayer to multilayer configurations.

To facilitate practical application, we developed a graphical user interface (GUI) that enables realtime data acquisition from a microscopic camera. This interface effectively applies the trained model to produce predictive outputs based on the acquired images. The process begins with the microscope scanning a substrate chip coated with a MoS2 film synthesized through CVD (Chemical Vapor Deposition), followed by image capture and processing. The resulting optical images serve as input for our model, which generates predictive outcomes that are further analyzed using histogram techniques to establish a layer distribution profile.

This innovative approach aims to propel materials science research forward and enhance the exploration of the unique properties of 2D materials, thus opening new avenues for their application in various technological domains.

#### Type of presence

Presence online

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Presenter: BABICHUK, Ivan (Wuyi University)

Session Classification: Advanced Optical Systems: From Design to Construction

Type: Oral

## Visualization of Radiation Intensity Distribution in Space Using Augmented Reality

Friday, November 8, 2024 6:05 AM (10 minutes)

In recent years, the use of radiation has been increasing in various fields. However, because radiation is invisible, it is difficult to tell which places have high radiation doses and which places have low doses. Therefore, there is a risk of exposure when using radiation.

In this research, we conducted a basic experiment to visualize the radiation intensity distribution in space using AR (augmented reality) technology. We installed RI (radio isotope) and shielding objects in the space and measured the non-uniform radiation distribution. Furthermore, the measured radiation intensity distribution was superimposed on real space using AR (augmented reality) technology. However, humans perceive visual information as two-dimensional image data. Therefore, we created a display that changes the displayed part depending on the time. Based on the acquired distribution data, a sphere was superimposed on the measurement location, and the color of the sphere changed depending on the intensity of the dose. At that time, by sequentially displaying information from the front to the back according to the passage of time, the observer can observe the information on the back side without being obstructed by the information on the front side, and it is possible to express it in a way that shows the overall distribution.

#### Type of presence

Presence online

Primary author: KAWAKAMI, Takumi (静岡大学)

Presenter: KAWAKAMI, Takumi (静岡大学)

Session Classification: Imaging Techniques, CT Imaging, and Augmented Reality

Type: Invited Talk

## POLYX@SOLARIS: layout, specification & first results

Monday, November 4, 2024 10:55 AM (20 minutes)

PolyX (polychromatic X-rays and polycpaillary X-ray optics) is a newly developed bending magnet beamline at SOLARIS National Synchrotron Radiation Centre in Kraków, Poland. SOLARIS is a 1.5 GeV synchrotron (circumference 96m) build with unique collaboration between MAX IV Laboratory and Jagiellonian University [1]. The beamline is dedicated to X-ray microimaging and X-ray spectromicroscopy [2] and is open for regular users since 1st March 2024.

PolyX offers several techniques:  $\mu$ CT ( $^{\circ}0.7\mu$ m resolution),  $\mu$ XRF,  $\mu$ XAS and  $\mu$ XES [3]. Imaging resolution  $^{\circ}200$  nm will be possible via recently developed X-ray tomography with multiple ultranarrow cone beams [4]. The end station can be easily reconfigured; therefore, in addition to implementing other synchrotron methods at short notice, PolyX will also work as a test station for innovative hard X-ray methods or new solutions of X-ray optics, new imaging geometries or detection systems. PolyX can also provide a dedicated area for user experiments and/or user endstations. The beamline operates in three modes: high flux (DMM, bandwidth 2 $^{\circ}$ ), high resolution (DCM, Si(111), bandwidth 0.02 $^{\circ}$ ) and a white beam mode. Polycapillary and monocapillary optics are used to generate hard X-ray beam in the energy range of 5-15keV with spot sizes in range  $^{\circ}5\mu$ m-100 $\mu$ m.

In this contribution the current status of the beamline will be presented as well as the beamline layout (optical, acquisition and detection systems). Additionally, first, commissioning results will be presented, to give an overall view on the beamline capability.

#### Type of presence

Presence online

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Presenter: Dr SOWA, Katarzyna (SOLARIS National Synchrotron Radiation Centre)

**Session Classification:** Unifying Efforts: Developing the Ukrainian Synchrotron Community and Research Infrastructure

Track Classification: USyNC Workshop

Type: Poster

## Study of noncovalent interactions in various solutions of thiophene-2-carboxylic acid

Friday, November 8, 2024 5:16 PM (3 minutes)

This research aims to investigate noncovalent interactions in various thiophene-2-carboxylic acid (TCA) solutions through experiments and simulations. Raman and infrared (IR) spectroscopy were utilized to analyse the vibrational characteristics of TCA in various solvent solutions. Experimental data analyzed using computing approaches include highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) frontier molecular orbitals, molecular electrostatic potential (MEP) mapping, and Mulliken charge distribution assessments. These analyses revealed vital information on TCA's electrical structure and propensity for noncovalent interactions. Noncovalent interactions, such as hydrogen bonding, van der Waals interactions, and p-p stacking, were investigated further using the noncovalent interaction index (NCI) and reduced density gradient (RDG) approaches, which identify the presence and type of weak interactions in molecular clusters. Electron localization function (ELF) and localized orbital occupier (LOL) analyses were utilized to study the electron localization and binding areas of TCA and its solvent complexes, providing more insight into binding behaviour. The results reveal that solvent polarity has a major effect on noncovalent interactions, as seen by shifts in vibrational frequencies and changes in the molecule's electrical environment. A combined experimental and computational investigation yields a comprehensive understanding of how noncovalent interactions influence molecular behaviour in solution. This study emphasizes the significance of these interactions in defining the chemical and physical properties of thiophene-2-carboxylic acid in a variety of environments, as well as providing useful insights for future chemistry and material science applications.

#### Type of presence

Presence online

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Presenter: KHUDAYKULOV, Bekzod (Samarkand State University)

Type: Oral

# Photoacoustic technique for determining optical absorption coefficients in nanostructured silicon

Thursday, November 7, 2024 11:55 AM (15 minutes)

Silicon nanowires have unique thermophysical and optical properties that suit various applications, including sensors, energy systems, and semiconductor industries. The optical properties of silicon nanowires can vary significantly depending on their synthesis method and the initial parameters of the crystalline material, both of which have a substantial impact on the resulting morphology. Consequently, developing reliable, non-destructive methods for measuring these optical characteristics is a crucial objective.

This report introduces an alternative approach to measuring the optical properties of silicon nanowire arrays with varying morphological characteristics, utilizing the photoacoustic gas-microphone method. The analysis is based on data from optical reflectance measurements performed using an integrating sphere, combined with thermal conductivity data derived from Raman spectroscopy. Light absorption in the samples was examined using photoacoustic methods, where the samples absorbed non-stationary laser radiation at multiple wavelengths within the visible spectrum. The amplitude-frequency dependence of the photoacoustic signal was analyzed, and a theoretical model was applied to approximate the experimental data, yielding values for the optical absorption coefficients of silicon nanowires with different morphologies.

This approach highlights the effectiveness of the photoacoustic method in evaluating the optical properties of silicon nanowires with different morphologies, offering a reliable and non-destructive means of analysis.

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#### Type of presence

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Session Classification: Advances in Nonlinear Optics and Laser-Matter Interactions

Type: Oral

## About the possibility of visualizing scattering areas of a medium using random lasing

Thursday, November 7, 2024 2:15 PM (15 minutes)

This work investigates random lasing (RL) in confined clusters of strongly scattering media using Monte Carlo method (MCM). The study include calculations of the photon distribution for both pumping and RL within such clusters, as well as the visualization of media containing these clusters.

The MCM demonstrates that the maximum photon density of RL is concentrated at the center of the clusters and gradually decreases toward the edges. This behavior is characteristic of confined scattering areas with a uniform particle distribution.

The calculations also highlight the importance of considering boundary reflection in such clusters, which influence the photon distribution. Boundary reflectivity partially smooth out the photon density distribution increasing it toward the edges, though the most significant effect is observed with decreasing cluster size. However, the multiple scattering at internal structure of the cluster plays the most crucial role, where it retains RL radiation and contributes to the formation of a central photon density maximum.

Computational results show that clusters can be clearly visualized due to multiple scattering when they illuminated by intense pump radiation, producing an RL photon distribution that can be used for imaging heterogeneous objects. This opens new possibilities for producing detailed images of complex media, such as biological tissues or other non-uniform systems.

By combining the computing of RL energy distribution within confined regions and its impact on visualization, this research provides new tools for simulating and optimizing RL in heterogeneous media. The results may find applications in various fields, including biomedical research and optical technologies.

#### Type of presence

Presence at Taras Shevchenko National University

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Session Classification: Advances in Nonlinear Optics and Laser-Matter Interactions

Type: Oral

## Enhancing Microfluidic Mixing Efficiency: CFD Analysis of a 3D Y-Shaped Serpentine Device

Friday, November 8, 2024 12:50 PM (15 minutes)

Microfluidic devices have attracted significant attention in various scientific and industrial applications due to their precise control over small amounts of fluids. This study employs Computational Fluid Dynamics (CFD) to investigate and evaluate the mixing efficiency within a three-dimensional (3D) Y-shaped serpentine microfluidic device. The device is designed to mix two different fluids, water and ethanol, at different flow rate values. The results demonstrated that low flow rates have greater mixing efficiency at the first units of the mixer than higher flow rate values, and mixing ethanol is slightly easier due to slower residence time. The results of this research provide valuable insights into the mixing efficiency of the microfluidic device and contribute to a comprehensive understanding of the impact of various operational parameters on the mixing process. Keywords: Microfluidics, micromixer, Computational Fluid Dynamics (CFD), lab on chip, pressure drop.

#### Type of presence

Presence online

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Presenter: EL MOUDEN, Zahra (Hassan II University ,Casablanca Morocco)

Session Classification: Advanced Optical Systems: From Design to Construction

Type: Oral

## Fluorescence based explosives sensor: potential of plasmonic enhancement for the development of ultrasensitive portable technique

*Friday, November 8, 2024 10:50 AM (15 minutes)* 

The global problem associated with the growth of terrorism has significantly worsened in the conditions of war in Ukraine due to the large-scale contamination of soil and water resources with explosives and explosion products. This makes the development of a sensitive, fast, cheap, portable and mass-producible sensor for the detection of explosives an urgent issue.

A number of attempts have been made to solve the problem of developing such a sensor using various recognition elements and sensor principles, including optical, electrochemical, surface-acoustic and immunological methods. Also, plasmonic enhancement is a well-known method of improving the sensitivity of optical sensors [1].

We propose to implement the optical method of fluorescent detection of explosives in a portable version with sensitive sensor elements in the form of composite materials with plasmonic nanostructures. Previous experience in the development of nanochip technology with a molecularly imprinted polymer coating for the detection of chemical analogs and taggants of explosives based on localized surface plasmon resonance [2, 3] and a highly selective aflatoxin sensor based on plasmon-enhanced fluorescence [4] will be used.

Therefore, the development of a portable sensor based on plasmon-enhanced fluorescence using molecularly imprinted polymers to ensure the selective detection of explosive nitro compounds and/or their chemical analogues in the gas and liquid phase with a sensitivity that allows the registration of picomoles (nanograms) or less of the specified substances with a response time of several minutes looks promising.

This work was supported by the National Research Foundation of Ukraine, project 2023.04/0057.

- 1. Li, M., Cushing, S. K., & Wu, N. (2015). Plasmon-enhanced optical sensors: a review. Analyst, 140(2), 386-406.
- V.I. Chegel, A.M. Lopatynskyi, V.K. Lytvyn, P.V. Demydov, J.P. Martínez-Pastor, R. Abargues, E.A. Gadea, S.A. Piletsky. Localized surface plasmon resonance nanochips with molecularly imprinted polymer coating for explosives sensing // Semiconductor Physics, Quantum Electronics & Optoelectronics. –Vol. 23. –2020. –pp. 431-436.
- E. Aznar-Gadea, P. J. Rodríguez-Canto, J. P. Martínez-Pastor, A. Lopatynskyi, V. Chegel, R. Abargues. Molecularly imprinted silver nanocomposites for explosive taggant sensing // ACS Applied Polymer Materials. –Vol. 3. –2021. –pp. 2960-2970.
- T. Sergeyeva, D. Yarynka, V. Lytvyn, P. Demydov, A. Lopatynskyi, Y. Stepanenko, O. Brovko, A. Pinchuk, V. Chegel. Highly-selective and sensitive plasmon-enhanced fluorescence sensor of aflatoxins // Analyst. –Vol. 147. –2022. –pp. 1135-1143.

#### Type of presence

Presence at Taras Shevchenko National University

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**Presenter:** Dr LOPATYNSKYI, Andrii (V.E. Lashkaryov Institute of Semiconductor Physics NAS of Ukraine)

Session Classification: Luminescent Materials and Photonic Applications

Type: Oral

## Laboratory X-ray spectroscopy and imaging as a preliminary step towards synchrotron experiments

Monday, November 4, 2024 11:35 AM (15 minutes)

X-ray spectroscopy experiments often require high-brilliance sources of X-ray radiation, provided by synchrotron or X-ray free electron laser (XFEL) facilities. However, acquiring access to such facilities is a complex procedure, which involves proposal application, long wait for the beamtime and travel expenses. Recent advances in the compact X-ray sources allowed for development of laboratory X-ray spectroscopy setups. While being orders of magnitude less brilliant compared to large facility sources, modern X-ray tubes with built-in focusing optics enable measurements of Xray absorption (XAS) and X-ray emission (XES) spectra in the laboratory environment. Despite the significant drawbacks (i.e. long acquisition times, limited energy range and noisy data), laboratory X-ray setups are a valuable research tool due to relatively low cost and practically unrestricted accessibility.

Herein, we report on development of laboratory setup for simultaneous acquisition of XAS, XES and X-ray fluorescence (XRF) data. Double von Hamos geometry-based spectrometer configuration allows for simultaneous XAS/XES measurements. On the other hand, the three-axis positioning stage enables XRF imaging and aids sample positioning. The setup is routinely used for the studies of electronic and structural properties of metal complexes, nanoformulation and biological samples.

#### Type of presence

Presence online

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**Presenter:** Dr YAKOVLIEV, Artem (Institute of Nuclear Physics, Polish Academy of Sciences, Krakow, Poland)

**Session Classification:** Unifying Efforts: Developing the Ukrainian Synchrotron Community and Research Infrastructure

Track Classification: USyNC Workshop

Manipulating over reflection, pol ...

Contribution ID: 69

Type: Invited Talk

# Manipulating over reflection, polarization and collection of light with metasurfaces

Thursday, November 7, 2024 3:45 PM (30 minutes)

Two-dimensional (2D) materials offer unique opportunities for photodetection, light emission, energy harvesting, and enhanced light-matter interactions. Even more interest brings the artificially engineered 2D micro- and nanostructures with on-demand properties paving the way towards a plethora of specific applications and devices including lensing, holography, imaging, polarimetry, biosensing, etc. The rapidly developing use of 2D nanostructures poses new challenges for their proper engineering and novel applications.

Here, we focus on plasmonic and dielectric metasurfaces, which are the periodic arrays of subwavelength scatterers. We study the properties of metasurfaces and their applications for (i) Brewster's angle shifting [1], (ii) surface waves routing [2], (iii) planar waveguide polarizer, (iv) anti-reflective coatings for solar cells, and (v) efficient light collection into optical fiber [3].

References

- [1] O. Yermakov, Physical Review A, 109(3), L031502 (2024).
- [2] O. Yermakov et al., Physical Review X, 11(3), 031038 (2021).
- [3] O. Yermakov et al., Applied Physics Reviews, 10(1), 011401 (2023).

#### Type of presence

Presence at Taras Shevchenko National University

Primary author: YERMAKOV, Oleh (Leibniz Institute of Photonic Technology)

**Presenter:** YERMAKOV, Oleh (Leibniz Institute of Photonic Technology)

Session Classification: Advances in Metasurfaces and Plasmonic Nanostructures

Type: Oral

## 3D semiconducting hybrid perovskites with aziridinium cation

Tuesday, November 5, 2024 10:15 AM (15 minutes)

The study of hybrid organic-inorganic perovskites has rapidly emerged as one of the fastest-growing research areas in materials science over the past decade. Our study shows that aziridinium cation (AzrH) is able to support 3D perovskite structure of (ArzH)PbHal3 (Hal = Cl, Br, I). Highly reactive species of aziridinium was stabilized in 3D lead halide frameworks and was found to be a small enough organic cation to promote the formation of semiconducting organo-inorganic materials. Bandgaps of 2.99 eV (Cl), 2.27 eV (Br) and 1.52 eV (I) were determined from Tauc plots.[1] Moreover, we have managed to obtain new 3D lead-free tin-based hybrid perovskites with aziridinium cation (AzrH)SnHal3 (where Hal = Cl, Br or I) which were also found to be semiconductors with narrow optical bandgaps.[2] As well, the possibility to fine-tune the bandgap of obtained perovskites through mixing halogen or Sn/Pb sites was investigated.

Additionally, by employing the antisolvent precipitation technique and stabilization with a cationic surfactant we succeeded in obtaining quantum dots of (ArzH)PbBr3 with average size 8.6 nm that display green (520 nm) luminescence.[3] Spin-coating was used to deposit aziridinium perovskite thin films.

Thus, the discovered compounds form a new group of 3D semiconducting perovskites that can widen the range of suitable materials for solar cells and light-emitting diodes production.

- 1. Petrosova, H. R. et al. Chem. Commun. 2022, 58, 5745-5748.
- 2. Kucheriv, O. I. et al. Inorg. Chem. Front. 2023, 10, 6953-6963
- 3. Semenikhin, O. A. et al. Chem. Commun. 2023, 59, 3566-3569.

#### Type of presence

Presence online

Primary author: Dr GURAL'SKIY, Il'ya (Taras Shevchenko National University of Kyiv)

**Co-authors:** Mr HALELUK, Dmytro; Ms PETROSOVA, Hanna; Mr SEMENIKHIN, Oleksandr; Dr KUCHERIV, Olesia; Dr SHOVA, Sergiu; Mr SIRENKO, Valerii

Presenter: Dr GURAL'SKIY, Il'ya (Taras Shevchenko National University of Kyiv)

Session Classification: Workshop on Sustainable Materials and Technologies

Track Classification: Workshop on Sustainable Materials and Technologies

Type: Oral

# Chiral 2D hybrid perovskites with amino acid cations

Tuesday, November 5, 2024 10:30 AM (15 minutes)

Layered 2D hybrid organic-inorganic perovskites (2D-HOIPs) exhibit a distinctive array of properties, including remarkable structural flexibility, enhanced resistance to moisture, and optoelectronic characteristics valuable for practical applications. Chiral HOIPs can widen the scope of possible applications towards detection and generation of circularly polarized light. We developed a series of new lead and tin-based 2D hybrid perovskites with cations of chiral α-amino acids: L-alanine,1 L-proline2 and L-histidine3. All obtained perovskites create layered structures in which inorganic layers are formed with MHal6 (M = Pb or Sn) octahedra connected in cornerof edge-sharing manner and are interleaved by organic layers established by amino acid cations. Chiral cations provide a breaking of spatial parity of these perovskites that results in their noncentrosymmetric crystal structures. The obtained chiral perovskites are semiconductors and display pronounced photoluminescence. Obtained (L-histidinium)2SnI4 has a remarkably low for 2D perovskites bandgap of 1.82 eV. As a "proof-of- concept", we created a prototype HOIPs photodetector. For the obtained prototype, light detection is observed in the wide range covering UV, visible and near-IR regions, marking a record achievement for 2D-HOIPs. Beyond photodetectors, these new perovskites hold promise for applications in various other optoelectronic devices, including solar cells, photodiodes, phototransistors, polarized light detectors, and more.

1 V. Y. Sirenko et al. New J. Chem., 2021, 45, 12606–12612.

2 V. Y. Sirenko et al. Dalt. Trans., 2023, 52, 10545–10556.

3 V. Y. Sirenko et al. Appl. Mater. Today, 2024, 41, 102452.

### Type of presence

Presence at Taras Shevchenko National University

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Presenter: Ms KUCHERIV, Olesia I. (Taras Shevchenko National University of Kyiv)

Session Classification: Workshop on Sustainable Materials and Technologies

Track Classification: Workshop on Sustainable Materials and Technologies

Type: Poster

# Green body composition for layered ceramic composites

Friday, November 8, 2024 4:27 PM (3 minutes)

Multilayer ceramics have the potential to replace monolithic ceramics due to their improved mechanical properties, including increased hardness, durability, and fracture toughness. The diverse loading conditions faced by structural materials require the development of customized layered structures for specific applications. A key advantage of layered ceramic composites is their ability to exhibit customized properties. Combining layers of different materials can optimize composites for specific mechanical, thermal, and electrical characteristics, enhancing performance in various environments. The use of layered composites can significantly improve the strength-to-weight ratio, which is crucial in industries such as aerospace and automotive.

Despite their advantages, layered ceramic composites face several challenges. The inherent brittleness of their components increases the risk of sudden failure under high mechanical stress, which limits their use where high fracture toughness is required. In addition, these materials are sensitive to sudden temperature changes, which can lead to thermal shock. The complexity of production is another issue. The production of layered ceramic composites involves complex processes of layer formation and sintering of raw materials, which require specialized equipment and expertise, which increases production costs and requires strict quality control.

In our study, we studied green body layering methods and advanced sintering techniques to create layered composites. Chosen method involves mixing the starting powder with a plasticizer solution, followed by reactive sintering. Various solutions were investigated. Tests have shown that some solvents can create excessive porosity, which impairs functionality. Therefore, petroleum solvent rubber was chosen because of its ability to dry at room temperature and its low level of impurities, ensuring that there is no negative impact on the sintering or compaction process. The microstructure of the resulting sample was further investigated.

This research has been supported by the National Research Foundation of Ukraine (Grant No. 2023.04/0139)

### Type of presence

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Presenter: Mr KLENIN, Mykola (Taras Shevchenko National University)

Type: Oral

# Quantum light in atmospheric turbulence

Friday, November 8, 2024 9:05 AM (15 minutes)

Quantum communication is a rapidly developing field focused on enhancing the security of communication protocols and new methods of information exchange. These techniques use quantum light propagating through glass fibers or free space as the information carrier. While the free-space channels are useful in many practical scenarios, they face challenging problems due to fluctuations in the refractive index caused by atmospheric turbulence.

We have tailored a numerical method from classical optics to study the effect of atmospheric turbulence on the quantum states of light [1]. This method employs the phase screen approach with the sparse spectrum model to simulate the complex propagation dynamics. Our method enabled us to validate existing analytical models of atmospheric quantum channels and to highlight limitations in the standard interpretation of their applicability. In particular, we showed that turbulence strength alone is not sufficient to determine model applicability, such that receiver aperture size must also be considered as a primary factor. In addition, we proposed a new heuristic analytical model based on the Beta distribution. This model showed better agreement with numerical simulations in almost the entire range of channel parameters. We also studied the time correlations [2], which provided insight into the preservation of continuous and discrete variable entanglement between two pulses in turbulent conditions, and estimated the possibility of preserving nonclassicality of quantum states with the method of adaptive selections.

[1] M. Klen and A. A. Semenov, PRA 108, 033718 (2023).

[2] M. Klen, D. Vasylyev, W. Vogel, A. A. Semenov, PRA 109, 033712 (2024).

### Type of presence

Presence at Taras Shevchenko National University

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Session Classification: Quantum Optics and Photonic Information Processing

Type: Poster

### Optical Band Gap Tuning in Mixed B-site and X-site Aziridinium Perovskites

Friday, November 8, 2024 4:30 PM (3 minutes)

Three-dimensional hybrid perovskites containing the aziridinium cation (AzrH)BX3 (where AzrH = aziridinium, B is Pb2+ or Sn2+ and X = Cl–, Br–or I–) exhibit semiconductive properties, making them suitable candidates for photovoltaic applications. Small changes in the composition of perovskites are shown to have a defining impact on optoelectronic properties of the reported materials. This study reports the possibility of optical band gap fine-tuning through mixing metals ((AzrH)PbxSn1-xBr3 series) or halogens ((AzrH)PbBrxI3-x series). All the obtained mixed perovskites crystallize in the Pm3<sup>-</sup>m space group at room temperature saving their 3D structure. The optical band gap of mixed-metal perovskites varies non-linearly from 1.96 eV to 2.46 eV, while halogen substitution tunes the band gap within the 1.57 –2.23 eV range, as measured by electronic spectroscopy. Additionally, phase transitions and powder X-ray diffraction were used to characterize the structural properties of these compounds. The results expand the scope of hybrid perovskites with tunable band gaps beyond conventional methylammonium and formamidinium-based systems, introducing a new series of metal-halide hybrids with potential applications in photovoltaic and optoelectronic technologies.

### Type of presence

Presence at Taras Shevchenko National University

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Presenter: PETROSOVA, Hanna (Taras Shevchenko National University of Kyiv)

Type: Poster

# QUANTUM CHEMICAL CALCULATIONS OF CHEMICAL BOND DEVIATION IN CLO2

Friday, November 8, 2024 5:19 PM (3 minutes)

In many small molecules the direction of the chemical bond, defined as the direction of the greatest change in the molecule's energy, appears not to coincide with the segment connecting the nuclei in a molecule. This phenomenon, first described in [1], is referred to as chemical bond deviation and has been thoroughly examined using classical 3N matrix method, e.g. [2], and ab initio methods, e.g. [3]. The present paper describes the quantum chemical calculations applied to determine the chemical bond deviation in ClO2 molecule. Hartree-Fock and DFT calculations were performed with Orca 5.0 software [4]. The chemical bond deviation angle  $\Delta$  appears to be small, about 0.7 degrees. This is a fairly predictable value, keeping in mind the small (relative to water) dipole moment of ClO2. The obtained information can be utilized in further research focusing on the interaction of the ClO2 with various surfaces.

- 1. Bilyu M.U., Okhrimenko B.A // Ukrainian Journal of Physics. 1999. vol. 44. №3. P. 326.
- 2. Komyshan P.N., Okhrimenko B.A., Yablochkova K.S.// Ukrainian Journal of Physics. 2014. Vol. 59(1). P.9
- Danylo, R.I, Okhrimenko B.A., Yablochkova K.S. // Photonic and Phononic Properties of Engineered Nanostructures V. 2015. Vol.9371 P.199
- 4. Neese, F. // Wiley Interdisciplinary Reviews: Computational Molecular Science. 2022. 12(5), e1606.

### Type of presence

Presence online

**Primary authors:** FURMAK, Illia (student); Dr YABLOCHKOVA, Kateryna (Associate Professor of the Department of Optics)

**Presenter:** FURMAK, Illia (student)

Type: Oral

# Peculiarities of forced radiation formation in thin dyed hybrid organic-inorganic films

Thursday, November 7, 2024 2:30 PM (15 minutes)

The development of integrated optoelectronics requires the creation of lasers with minimum sizes which would be acceptable for integration into the corresponding optoelectronic circuits. The most suitable for this purpose are waveguide planar lasers, which are integrated with waveguides and other devices of the optoelectronic circuit. At present, most attention is paid to films based on rare earth ions in glass and crystal matrices and lasing dyes in polymers with a refractive index in the range from 1.3 to 1.6.

We have investigated the features of the occurrence of Rhodamine 6G stimulated emission in hybrid organic-inorganic films (Pluronic 123 + TiO2 or SiO2) with a minimum thickness close to the critical value of the waveguide mode. The inorganic component of the film provided a variation of the refractive index in the range of 1.49 - 1.565, while the organic component allowed the introduction of a dye of high (up to several mmol/l) concentration. The films were placed on the glass substrate by dipping (deep coating) and spin coating technique, which made it possible to obtain films with thicknesses greater and less than the critical one, respectively. The pumping was performed by the second harmonic of the YAG:Nd3+ laser.

When the threshold pumping intensity of 0.14 MW/mm<sup>2</sup> was exceeded in TiO2-based films with a thickness of 340 nm by 10% above the critical value (300 nm), a rapid narrowing of the radiation spectrum from 60 to 5 nm and the appearance of a directed coherent beam with an angular divergence of 6.3° were observed. The beam had a pronounced interference structure on the side of the substrate, indicating that a part of the beam penetrated it. The small divergence compared to the diffraction divergence at the film end confirms that the radiation formation is influenced by the substrate, which is thicker (1 mm). The formation of interference strips can be associated with the emergence of Lummer-Herke modes, which are formed when radiation partially penetrates into the substrate when incident on it at an angle slightly less than the critical one. At thicknesses less than the critical one, no such effects occurred.

### Type of presence

Presence at Taras Shevchenko National University

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**Presenter:** Mr PODSHEBIAKIN, Artem (Taras Shevchenko National University of Kyiv)

Session Classification: Advances in Nonlinear Optics and Laser-Matter Interactions

Tight tests for nonclassicality

Contribution ID: 77

Type: Oral

# **Tight tests for nonclassicality**

Friday, November 8, 2024 8:35 AM (15 minutes)

An optical state is considered nonclassical if its density operator cannot be represented as a statistical mixture of coherent states. This definition renders prominent phenomena such as sub-Poissionian statistics of photon counts or quadrature squeezing nonclassical. However, determining whether an optical state is nonclassical is a challenging task since it requires tomographic reconstruction of its density operator. A more practical approach is to understand whether given measurement statistics could be in principle simulated by a mixture of coherent states.

The detection of nonclassicality of measurement statistics is still a nontrivial task. Mathematically, a set of all classical statistics for a given set of measurements represents a convex hull of statistics exhibited by coherent states. This enables one to apply hyperplane separation theorem in order to test nonclassicality of measurement statistics. Each direction in the space of statistics is considered a normal of a hyperplane that touches the convex hull and divides the space into two parts. If statistics under consideration is not in the same halfspace as the hull, one can conclude that it is nonclassical.

Considering all possible directions in the statistics space can be a computationally expansive task. Fortunately, one can identify a minimal set of useful directions such that all other directions need not be considered in order to determine nonclassicality. Each direction corresponds to a tight inequality whose violation implies nonclassicality. [1]

[1] V. S. Kovtoniuk, et al., PRA 109, 053710 (2024)

### Type of presence

Presence at Taras Shevchenko National University

Primary author: KOVTONIUK, Vadym (Bogolyubov Institute for Theoretical Physics)

Presenter: KOVTONIUK, Vadym (Bogolyubov Institute for Theoretical Physics)

Session Classification: Quantum Optics and Photonic Information Processing

Type: Invited Talk

### Scanning Probe Lithography and Laser-Assisted Direct Nano-Relief Engineering

Wednesday, November 6, 2024 9:20 AM (20 minutes)

Scanning Probe Lithography (SPL) is a versatile technique for prototyping planar nanostructures with simultaneous in situ characterization. Using a nanoscale tip, surfaces can be mechanically or electrically modified to create predefined patterns, either through direct modification or thin resist layer masks. Additionally, interference and plasmon lithography allow for the efficient generation of nanoscale patterns under SPM control.

Our approach has proven effective in fabricating molecular electronic device elements, including arrays of subnanometer threads and plasmon waveguides constructed from elastic linkers and gold nanocylinders. Furthermore, multilayer graphene flakes were precisely perforated, cut, and engraved using SPL.

In GeSn alloys, we achieved local electronic property modification by applying electric fields between the tip and the surface. The resulting variations in electronic work function and resistivity were linked to increased Sn content in the near-surface regions of the patterns created by the SPM tip.

We also investigated the kinetics of surface relief grating (SRG) formation in amorphous AsSe thin films. SRGs were induced using holographic recording with near-bandgap light and further enhanced with interference patterns. The growth kinetics were found to depend on film composition and light polarization. Sub-wavelength reliefs formed on the AsSe surface through interaction with an underlying gold pattern, leveraging localized near-field effects from surface plasmon resonance.

These findings demonstrate the potential of SPL and laser-assisted techniques for advanced nanoengineering and material property tuning at the nanoscale.

The work is supported by the National Research Foundation of Ukraine (2023.03/0060).

### Type of presence

Presence at Taras Shevchenko National University

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Co-author: KONDRATENKO, Serhiy

Presenter: Dr LYTVYN, Petro (V. Lashkaryov Institute of Semiconductor Physics NAS Ukraine)

**Session Classification:** Workshop on Direct Optical Lithography for Advanced Opto- and Microelectronics

Type: Poster

# Spontaneous and stimulated UV laser-induced excitonic luminescence from ZnO nanopowder

Friday, November 8, 2024 4:33 PM (3 minutes)

Zinc oxide (ZnO) is one of the best photoactive wide-gap metal-oxide semiconductor materials, whose optoelectronic properties are of great interest for nanophotonics [1,2]. In particular, photo excited ZnO exhibits strong excitonic UV photoluminescence (PL) at room temperature (RT). But despite all advances in ZnO nanophysics, some features of RT excitonic PL of ZnO nanoparticles (NP) are not so clear, especially in disordered nanostructures with random light scattering. We tried to study this issue in more detail. Experiments were carried out with finely dispersed ZnO powder of high-grade quality obtained by a hydrothermal method and characterized by XRD, Raman and UV-Vis spectroscopy. Measurements showed that ZnO NPs have a nodular shape with sizes from 1 µm to 100 nm and crystallites of ~20 nm. In the PL spectra excited in ZnO powder by a pulsed N2 laser at 337 nm, we observed a nonlinear amplification of excitonic UV PL emission at 387 nm and a decay of the visible PL emission at 500 nm. A superlinear increase in the intensity of the excitonic UV PL band with its narrowing with increasing excitation intensity indicates stimulated emission of ZnO NPs. This regime is realized over the entire excitation range due to non-resonant diffusion mode of light amplification, similar to random lasing in Letokhov-type scattering photonic media. Estimated gain is ~100 cm-1, threshold is ~1 mJ/cm2. Research is in progress.

A.Tashiro, Y.Adachi, T.Uchino, J.Appl.Phys. 133, 221101 (2023).
 H.Cao, Y.Eliezer, Appl.Phys.Rev. 9, 011309 (2022).

### Type of presence

Presence online

**Primary authors:** Dr IZMAILOV, Igor (V.E. Lashkaryov Institute of Semiconductor Physics, National Academy of Sciences of Ukraine); Dr NAUMOV, Vadym (V.E. Lashkaryov Institute of Semiconductor Physics, National Academy of Sciences of Ukraine); Dr FEDORENKO, Leonid (V.E. Lashkaryov Institute of Semiconductor Physics, National Academy of Sciences of Ukraine); Prof. YUKHYMCHUK, Volodymyr (V.E. Lashkaryov Institute of Semiconductor Physics, National Academy of Sciences of Ukraine)

**Presenter:** Dr IZMAILOV, Igor (V.E. Lashkaryov Institute of Semiconductor Physics, National Academy of Sciences of Ukraine)

Type: Poster

### Intermolecular interaction of (CH3)2CO•••HCl complex: IR spectra, DFT method, QTAIM, NCI, RDG, ELF, LOL, FMO analyses.

Friday, November 8, 2024 4:09 PM (3 minutes)

Infrared absorption spectra of free molecules (CH3)2CO/HCl and (CH3)2CO--+HCl complex are recorded in the 4000-400 cm-1 region with a Bruker IFS-125 Fourier spectrometer in gas state and with Kr, Xe solutions at different temperatures. In the free acetone and its complex with HCl, the spectral characteristics of the fundamental ranges Q(C=O),

, Q-(C-C), and vHCl are measured. Particular attention is paid to determining the effect of H-Cl and C=O on the bond length, frequency, and intensity in the (CH3)2CO···HCl complex. In the calculations, intermolecular interactions, anharmonic potential energy, and dipole moment surfaces are analysed using the DFT method based on the B3LYP/6-311++G(d,p) basis set. Topological (QTAIM, NCI, RDG, ELF, and LOL) studies are used to examine interactions (hydrogen bond and Van der Waals interactions) at the crucial locations of connections. Information on the HUMO-LUMO gap and other electronic characteristics is given. A good agreement is observed between experimental and theoretical results.

### Type of presence

Presence online

Primary author: Ms NURMURODOVA, Gulshan (Samarkand State University)

**Co-authors:** Mr KHUJAMOV, Utkir (Samarkand State University); Dr MURODOV, Gulamkhon (Samarkand State University)

Presenter: Ms NURMURODOVA, Gulshan (Samarkand State University)

European X-ray Free-Electron La ····

Contribution ID: 81

Type: Invited Talk

# European X-ray Free-Electron Laser: working principle and capabilities

Monday, November 4, 2024 1:30 PM (30 minutes)

Free-Electron Lasers are versatile research tools that provide powerful (up to TW-order) and short (down to sub-fs-order) X-ray pulses. European XFEL is an international facility dedicated to deliver such pulses to users

In this presentation I will introduce listeners to the basics of FEL Physics. We will discuss ca-

pabilities of the European XFEL facility in both nominal and special operation modes, such as self-seeding, 2-color generation and attosecond pulse production.

### Type of presence

Presence online

Primary author: Dr SERKEZ, Svitozar (European XFEL)

**Presenter:** Dr SERKEZ, Svitozar (European XFEL)

**Session Classification:** Exploring Ultrafast Phenomena with the XFEL: Instruments, Capabilities, and Applications

Type: Invited Talk

### Object detection by wide-field multi-camera optical systems followed by their tracking through narrow-field devices mounted on turrets

Friday, November 8, 2024 12:00 PM (20 minutes)

The paper is devoted to the development and research of hardware-software complex, computing methods and software for detecting missiles and UAVs using optical systems mounted on stationary platforms and support-rotating devices. The computational methods and software developed are designed to address the detection and tracking of target movement (trajectories) through optical systems, with an emphasis on adapting these methods to meet the evolving requirements of observation. The developed solutions enable the creation of an efficient multi-client network for detecting and monitoring various types of aircraft, including the ability to target them using laser systems mounted on support-rotating devices.

The development and research are based on computational methods from the CoLiTec and Lemur software, which has been implemented in the USA, Ukraine, Poland, Slovakia, Thailand, Argentina, and Kazakhstan. This software has facilitated the automated discovery of over 1,600 asteroids and 4 comets and is currently used for the automatic tracking of Earth's artificial satellites.

During the course of the work, several computational methods and software were developed and upgraded, including: transmission of images and streaming video; compensation for optical image distortion; identification of object types (circles/streaks) in frames; generation of typical forms in images when the form cannot be analytically determined; object detection using a matched filter (correlator) based on a non-analytically defined form; estimation of object position and brightness (fitting) with unknown shapes that cannot be analytically specified; detection of high-speed objects with unknown trajectories across a series of frames; and accumulation of image energy along unknown trajectories.

Methods and tools for generating and displaying the results of high-speed target detection, as well as methods and tools required for integration with automated support-rotating devices, were also developed.

### Type of presence

Presence at Taras Shevchenko National University

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Session Classification: Advanced Optical Systems: From Design to Construction

Type: Poster

### Optical Properties of Luminescent Centers in Bi-Doped Glass-Ceramics: A TD-DFT Study

Friday, November 8, 2024 4:36 PM (3 minutes)

Theoretical modeling of electronic structures of heterostructure composites is a powerful tool for developing novel optical materials. This work presents the results of calculations of the excited electronic states and optical spectra of  $MoO_4$  groups and Bi ions, considered potential luminescence centers in the glass-ceramic composite "KBi( $MoO_4$ )<sub>2</sub> crystal@phosphate-molybdate glass of  $K_2O-P_2O_5-MoO_3-Bi_2O_3$  system."

Atomic and electronic structures of the crystal, glass, and interphase layers were obtained using molecular dynamics and band-periodic density functional theory (DFT) methods. Geometry optimization was performed with the Gaussian software package. Excited electronic states were calculated using time-dependent DFT within a molecular cluster approach and the two-level ONIOM-2 method. The quantum mechanical (QM) region included the MoO<sub>4</sub> groups or Bi ions, while the mechanical (MM) region comprised all other atoms. Electronic embedding accounted for electrostatic interactions between QM and MM regions, treating QM atoms with TD-DFT and MM atoms as partial charges in the quantum-mechanical Hamiltonian.

Calculations were performed on ten structures of the glass and interphase regions, and results were averaged for statistical significance. Similar calculations were done for the  $MoO_4$  groups and Bi ions in the KBi( $MoO_4$ )<sub>2</sub> crystal. The results indicate significant differences in the optical absorption spectra of Bi atoms and  $MoO_4$  groups across different regions of the composite.

Comparisons of the optical spectra for the crystal, glass, and interphase components with experimental data highlight the unique properties of each component. The origin of intrinsic luminescence in phosphate-molybdate glass-ceramics is discussed.

### Type of presence

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Presenter: BORYSIUK, Viktor (Taras Shevchenko National University of Kyiv)

Type: Oral

# Application of textural analysis for research the relationship between the microrelief of surfaces and laser speckles

*Friday, November 8, 2024 11:20 AM (15 minutes)* 

This work investigates the use of texture analysis to establish a quantitative relationship between laser spot properties and the microrelief parameters of metal surfaces. Surface microreliefs, consisting of microscopic irregularities, play a crucial role in determining material properties. Analysis of these irregularities is crucial in materials science for predicting behavior, developing materials, and quality control. Traditional methods exist, but laser speckle interferometry offers a non-invasive, precise alternative. When a laser beam interacts with a rough surface, it is scattered, forming a spot pattern that encodes statistical information about the surface. Our study investigates whether this information can provide insights into the properties of microreliefs.

We analyzed seven metal samples and captured microscopic images using dark-field microscopy and speckle images using a special optical setup. Texture parameters such as fractal dimension, anisotropy, contrast, correlation, entropy and second angular momentum were calculated. The results showed a strong Pearson correlation between three key parameters: fractal dimension, anisotropy and entropy, which is consistent on both micrographs and speckle images.

This correlation implies that speckle texture analysis can effectively characterize the underlying microrelief of metal surfaces. The fractal dimension of speckles reflects the complexity of the surface, anisotropy indicates directional variations in roughness, and entropy captures the randomness of the surface texture. Our results suggest that speckle analysis can serve as a powerful tool to study and predict material properties, enabling non-invasive quality control and material design.

### Type of presence

Presence at Taras Shevchenko National University

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Session Classification: Luminescent Materials and Photonic Applications

Type: Oral

# Luminescent glass-ceramics and cellulose-oxide composites based on K2Eu(PO4)(WO4) red phosphor

*Friday, November 8, 2024 10:35 AM (15 minutes)* 

Elaboration of effective red phosphor for lighting applications remains one of the main directions in material science nowadays. Such phosphor should absorb part of ultraviolet or blue emission of the base chip and transform obtained energy into red light. Oxide compounds doped with rareearth ions, namely Eu<sup>3+</sup> ions, are among the candidates for such phosphors. It was found recently that K<sub>2</sub>Eu(PO<sub>4</sub>)(WO<sub>4</sub>) reveals intensive red luminescence under excitation at 380, 393, and 466 nm. Moreover, the studies showed that this material exhibit a quantum yield close to unity for abovementioned excitations. It is worth to note that covering of semiconductor chip with phosphor layer can be performed by introducing of the luminescent micro/nanoparticles in glass or polymer matrix. Consequently, glass-ceramics and oxide@polymer composites are formed. Interaction between introduced phase of oxide particles and the phase of the glass or polymer matrixes can be monitored by analysis of the luminescent characteristics changes.

In this work, the morphology and optical properties of K<sub>2</sub>Eu(PO<sub>4</sub>)(WO<sub>4</sub>) red phosphor, K<sub>2</sub>O-P<sub>2</sub>O<sub>5</sub>-WO<sub>3</sub>-Bi<sub>2</sub>O<sub>3</sub>-K<sub>2</sub>Eu(PO<sub>4</sub>)(WO<sub>4</sub>) glass-ceramics and K<sub>2</sub>Eu(PO<sub>4</sub>)(WO<su composites have been studied. The Eu3+ ions were used as structural probes due to a dependence of their luminescence properties on symmetry and composition of the nearest surrounding. Effects of interphases and interfaces formation on properties of the materials under study are discussed taking into account the results of optical and scanning electron microscopy, X-ray diffraction, infrared transmittance, diffuse reflectance, and photoluminescence spectroscopy. The studied glass-ceramics and cellulose-based composites have demonstrated perspectives for application as luminescent covers for WLEDs.

This work has received funding through the EURIZON project, which is funded by the European Union under grant agreement No.871072.

### Type of presence

Presence at Taras Shevchenko National University

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Presenter: Dr CHORNII, Vitalii (National University of Life and Environmental Sciences of Ukraine)

Session Classification: Luminescent Materials and Photonic Applications

Type: Oral

# A novel approach for the precise control of growth kinetics in GaN(0001) epilayers

*Tuesday, November 5, 2024 5:30 PM (15 minutes)* 

Gallium nitride (GaN) is a highly effective semiconductor for a wide range of applications, including light-emitting diodes (LEDs) and laser diodes (LDs) [1]. However, the thermal, optical, and electrical properties of GaN vary significantly depending on the deposition parameters employed. Temperature control at each stage of deposition, such as steady state, accumulation of Ga monolayers, formation of Ga droplets, consumption of Ga droplets, crystallization of residual Ga monolayers, and restoration of steady state, is particularly important. Here, we demonstrate the advantages of our approach, which allows us to monitor the growth kinetics of the GaN layer and accurately distinguish between the accumulation of metallic Ga and its crystallization into GaN during molecular beam epitaxy (MBE). We present a novel method for measuring nitrogen plasma flux based on the analysis of signal variations recorded by a pyrometer. Consecutive metallic gallium deposition and GaN crystallization on GaN (0001) substrates were performed using different nitrogen plasma fluxes. The data demonstrate two distinct linear behaviors of plasma flux in relation to the plasma generation parameters: inert nitrogen gas flux and RF power. This technique circumvents the need for additional external equipment like RHEED or complex optical spectrometers, making it adaptable for both MBE and Metal-Organic Chemical Vapour Deposition (MOCVD) systems.

All the authors acknowledge funds from the project ANTHEM 2022-NAZ-0488.

1. S. Sanguinetti, S.Bietti, N.Koguchi, Droplet Epitaxy of Nanostructures, Molecular Beam Epitaxy, Elsevier, 2018, Pages 293-314.

### Type of presence

Presence online

**Primary author:** Mr CANCIANI, Matteo (Università Milano-Bicocca)

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Presenter: Mr CANCIANI, Matteo (Università Milano-Bicocca)

Session Classification: Workshop on Sustainable Materials and Technologies

Track Classification: Workshop on Sustainable Materials and Technologies

Type: Oral

# Nanostructured InGaN for biomedical application

Friday, November 8, 2024 2:45 PM (15 minutes)

Epitaxial growth of GaN and InGaN heterostructures is very promising for biosensor applications due to their excellent chemical stability, biocompatibility with low toxicity to living cells, and high carrier mobility [1]. Compared to InN thin films, InGaN quantum dot (QD)-based biosensors demonstrate a twofold increase in sensitivity and a fivefold faster response. While significant progress has been made, optimization of InN QD deposition, InGaN growth, and sensor functionalization remains crucial for realizing wearable transdermal biosensors (WTBs). The InGaN nanostructured thin films were grown using Plasma-Assisted Molecular Beam Epitaxy (PA-MBE) on Si (111) substrates, enhancing the sensitivity of the biosensors. The growth mechanism and geometrical properties of the InGaN nanocolumns were investigated using scanning electron microscopy. Structural characterization and accurate surface morphology analysis were performed. We investigated the variation in nanocolumn shape, density, and diameter as a function of the In/Ga ratio, which was controlled by deposition parameters. We show that achieving high indium content (40-50%) is critical for maximizing surface state energy and enabling ohmic contact between p-type Si and n-type InGaN. Nanostructured InGaNs are promising as a platform for biosensors functionalized with disease-specific antibodies dissolved in hydrogels to recognize target proteins, with a redox reaction indicating their presence.

All the authors acknowledge funds from the project ANTHEM: 2022-NAZ-0488. 1. M. Azadmand et al., Nanomaterials (Basel) 3,12 (2022) 3887.

### Type of presence

Presence online

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**Presenter:** Dr KOPLAK, Oksana (Università degli Studi di Milano-Bicocca)

Session Classification: Biomedical Imaging and Nanotechnology

Type: Poster

# Isotope effects on the IR spectrum of the CX3Y•••HCl complex in liquefied argon: DFT calculations, topological analyses, and electronic properties

Friday, November 8, 2024 4:39 PM (3 minutes)

Infrared spectra (4000-400 cm-1) of free molecules CX3Y (X=H, D, Y=F, Cl, Br), HCl, and CX3Y•••HCl mixtures in liquefied argon (90, 100-120 K) are recorded. The intermolecular interactions of the CX3Y•••HCl complexes are studied using the DFT method based on the B3LYP/6–311++G(d,p) basis set. The effect of deuterium (D), an isotope of the hydrogen atom (H), on the vibrational spectra of hydrogen-bonded complexes is discussed. Harmonic and anharmonic vibration frequencies are determined in calculations. The intermolecular interactions in these complexes are studied for the first time using topological (AIM, NCI, RDG, ELF, and LOL) analyses. NBO analysis and Mulliken atomic charge distribution are used to study the charge transfer mechanism in intermolecular interactions. The HUMO-LUMO gap and MEP are used to determine the electronic properties. The good agreement shows between the experimental and theoretical results

### Type of presence

Presence online

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**Presenter:** Mr KHUJAMOV, Utkir (Samarkand State University)

Type: Invited Talk

# Synchrotron based search for new quantum materials

Monday, November 4, 2024 9:10 AM (25 minutes)

The electronic band structure holds the key to understanding the properties of quantum materials, as well as the mechanisms behind quantum phenomena like superconductivity and other electronic orderings. In this talk, I will briefly review our results in this area and highlight cases where synchrotron experiments play a crucial role in determining the real electronic band structure, thereby advancing the development of new quantum applications. I will also present our ongoing projects, including theory-assisted searches for novel materials and applications, such as a high-speed matrix kinetic detector based on multi-band superconductors.

### Type of presence

Presence at Taras Shevchenko National University

Primary author: Prof. KORDYUK, Alexander (Kyiv Academic University)

Presenter: Prof. KORDYUK, Alexander (Kyiv Academic University)

**Session Classification:** Unifying Efforts: Developing the Ukrainian Synchrotron Community and Research Infrastructure

Type: Oral

# Structural and optical properties of β-Ga<sub>2</sub>O<sub>3</sub> thin films obtained by spray pyrolysis

*Tuesday, November 5, 2024 4:05 PM (15 minutes)* 

Beta gallium oxide ( $\beta$ -Ga<sub>2</sub>O<sub>3</sub>) thin films have attracted considerable research interest due to their wide bandgap, high thermal and chemical stability, and high breakdown voltage making them suitable for power electronics, UV photodetectors, solar cells, and sensors [1]. In this work,  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> thin films were deposited on c-plane sapphire substrates via spray pyrolysis [2]. This approach is cost-effective and can be further used in large-scale production.

For spray pyrolysis, we used Ga(NO<sub>3</sub>)<sub>3</sub> dissolved in a 1 : 1 water-ethanol mixture or water with 1% polyethyleneimine (PEI), followed by annealing at 800 °C or 1000 °C. The films were characterized by SEM, AFM, XRD, Raman spectroscopy, spectroscopic ellipsometry, UV-vis. spectroscopy, and electrical resistance using the four-point probe. The films obtained are stoichiometric Ga<sub>2</sub>O<sub>3</sub> in the  $\beta$ -phase with thicknesses of ~70–100 nm (spray from precursor water-ethanol solution) and ~30 nm (water-PEI solution). The films revealed a preferred orientation ( $\overline{2}01$ ) in agreement with previous results for  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> on c-plane sapphire [3]. The samples showed high transparency in the visible range and a sharp absorption edge in the UV range with bandgaps of 4.9 to 5.3 eV. The resistivity of the undoped films was in the G\Omega range.

Thus, the current results show that spray pyrolysis allows the fabrication of highly crystalline, transparent, and dielectric  $\beta$ -Ga<sub>2</sub>O<sub>3</sub> films suitable for further studies as UV photodetectors.

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[3] Akazawa, Housei. Formation of various phases of gallium oxide films depending on substrate planes and deposition gases. Vacuum, 2016, 123: 8-16.

#### Type of presence

Presence online

Primary author: Ms SHAMROVSKA, Polina (Chemnitz University of Technology)

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Presenter: Ms SHAMROVSKA, Polina (Chemnitz University of Technology)

Session Classification: Workshop on Sustainable Materials and Technologies

Track Classification: Workshop on Sustainable Materials and Technologies

Type: Invited Talk

### Glass-ceramic and hybrid nanocomposites with luminescent complex oxide fillers: research and possible applications

Friday, November 8, 2024 10:00 AM (20 minutes)

This talk concerns research of optical nanoscale materials which are synthesized/manufactured by our research team in Kyiv, and are being researched in Ukraine and beyond. The history of these studies goes back 11 years, and it was preceded by the study of the inorganic molecular anions (MA) like XOnm- (X = S, Se, Te, Cr, V, Mo, etc) in frozen aqueous solutions. Then, there were studies of inorganic oxide heterodesmic crystals doped with MA, ions of rare earth (RE), and transition elements (TE). The experience allowed us to start elaborating on the composite materials containing nano/microparticles of the mentioned and similar types of crystals and MA.

Today, our research is focused on the glasses and glass ceramics made on the basis of simple oxides of alkali metals, boron, phosphorus, molybdenum, and tungsten. Another direction is the study of hybrid nanocomposites, where the matrix is fibrillated, nano-sized, or microcrystalline cellulose.

The elaborated composites possess both intrinsic and impurity short-decay and long-lasting luminescence caused by ions of heavy metals, RE, and TE located in the matrix or the filler: incorporated crystalline particles.

Hybrid composites, under certain conditions, also exhibit mechanoluminescent and piezoelectric properties.

Special attention is paid to the study of the influence of the interphase layers on the nanocomposites' properties. These layers are formed between the matrix and the filler by the interdiffusion of their atoms and molecules.

The research combines the synthesis/fabrication of composites, a wide range of experimental and theoretical calculations, and modeling.

### Type of presence

Presence at Taras Shevchenko National University

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Presenter: Prof. NEDILKO, Serhii (Taras Shevchenko National University of Kyiv)

Session Classification: Luminescent Materials and Photonic Applications

Type: Oral

# Theoretical modelling of luminescence processes in oxide glass-ceramic nanocomposite materials

Friday, November 8, 2024 10:20 AM (15 minutes)

The optical properties of glass-ceramic nanocomposite materials "oxide-glass matrix @ oxidecrystalline micro/nanoparticles filler" are now the subject of intensive research. The unique physical properties of such composites are determined by interphases regions, which have atomic structure and chemical composition intermediate between the crystalline and glass components. The atomic structure of interphases can be obtained in calculations by molecular dynamics (MD) methods. Further application of the electronic structure calculations allows to obtain the most important micro- and macro-characteristics of the interphase layers and thus to explain the experimentally observed properties of glass-ceramic composites.

This report presents results of complex computational and experimental studies of the atomic and electronic structures of luminescent oxide glass-ceramic composite materials. Three different types of glass-ceramic composited are considered: a) KBi(MoO4)2 crystal @ K2O-P2O5-MoO3-Bi2O3 glass b) K2Bi(PO4)(WO4) crystal @ K2O-P2O5-WO3-V2O5 glass; c) LaVO4 crystal @ Li2O-V2O5-B2O3 glass. The atomic structures of interphase regions were calculated by MD methods. The electronic structure calculations were performed in the DFT approximation using the band-periodic plane wave pseudopotential method. The excited electronic states and optical spectra of possible centers of luminescence of glass-ceramic composite materials are calculated using the Time-Dependent Density Functional Theory (TD-DFT) within molecular cluster approach.

Obtained computational results are compared with experimental data on structural analysis, optical and luminescence spectroscopy. The mechanisms of luminescence and excitation energy transfer in oxide glass-ceramics of different types are discussed.

### Type of presence

Presence at Taras Shevchenko National University

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Presenter: Dr HIZHNYI, Yuriy (Taras Shevchenko National University of Kyiv)

Session Classification: Luminescent Materials and Photonic Applications

Type: Poster

### Electronic structures and optical properties of different phases of polyvinylidene fluoride (PVDF) crystals

Friday, November 8, 2024 4:42 PM (3 minutes)

Polyvinylidene fluoride (PVDF) is an organic polymer that exhibits significant potential and commercial appeal for modern applications in nanotechnology, microelectronics, and biomedicine. A real PVDF polymer is almost always a mixture of several polymorphic phases that are difficult to separate. Determining the phase composition of PVDF mixtures is a critical technological task. This report presents results of the ab-initio calculations of the electronic band structures of the three most common phases of PVDF crystals:  $\alpha$ -,  $\beta$ -, and  $\gamma$ -PVDF. The results include the one-electron band structures (band dispersion curves), partial densities of electronic states, spatial distributions of electron density, spectra of dielectric constants, complex refractive indices, absorption and reflection spectra, infrared absorption, Raman scattering, and X-ray diffraction patterns for the  $\alpha$ -,  $\beta$ -, and  $\gamma$ -phases of PVDF. The analysis of the electronic structure calculations allowed to make several conclusions regarding the formation of electronic and optical properties of the  $\alpha$ -,  $\beta$ -, and  $\gamma$ -phases of PVDF, as well as predictions about the potential for experimental monitoring of the phase composition of this compound. It was established that detecting the simultaneous presence of  $\beta$ - and  $\alpha$ -(or  $\gamma$ -) phases in PVDF crystal samples can be effectively achieved using reflection spectroscopy in the vacuum ultraviolet range, infrared absorption, Raman scattering, and X-ray phase analysis. However, distinguishing the presence of the  $\alpha$ -phase against the background of the y-phase using these methods would be practically impossible.

### Type of presence

Presence at Taras Shevchenko National University

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Presenter: BARANCHICOV, Zahar (student)

Type: Invited Talk

# Optoelectronic Applications of Metal Halide Perovskites

Tuesday, November 5, 2024 9:00 AM (30 minutes)

Over the past decade, metal halide perovskites (MHPs)—a novel class of water-soluble semiconductors with an exceptional combination of unique properties—have garnered significant attention for their potential in a wide range of optoelectronic devices. These include solar cells, detectors for optical and ionizing radiation, light sources, lasers, and various optoelectronic sensors.

As direct-gap semiconductors, MHPs offer high charge carrier mobility and confinement, along with the ability to tune their bandgap. This tunability enables the development of novel optical imaging arrays with up to three times the efficiency and resolution of current technologies, along-side superior color recognition and the elimination of geometric artifacts such as demosaicing [1]. The high atomic charge of MHPs, combined with their solution-processable nature, makes them particularly suitable for creating low-cost, efficient detectors for ionizing radiation. These materials allow for the combination of simple growth and deposition techniques for active layers with the ability to count single photons, making them highly effective for advanced detection applications [2-4].

Furthermore, MHPs'tolerance to defects in their electronic structure leads to a high quantum yield, making them ideal for next-generation dipoles. Additionally, their excitonic properties, present even at room temperature in low-dimensional films, open up possibilities for use in optical amplifiers and lasers [5].

In low-dimensional MHPs, the lattice's softness results in self-trapped excitons, which exhibit extreme sensitivity to external factors like temperature and pressure. This characteristic paves the way for developing high-performance phosphors for applications in thermography [6] and tensography.

The unique properties of metal halide perovskites make them highly promising materials for creating optoelectronic devices with advanced capabilities. Moreover, they offer exciting possibilities for inventing new types of sensors and functional devices with enhanced performance.

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### Type of presence

Presence online

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Session Classification: Workshop on Sustainable Materials and Technologies

Track Classification: Workshop on Sustainable Materials and Technologies

Type: Invited Talk

### Dopant-induced effects in zirconia-based materials: interrelation between structural transformation and luminescence variation

Monday, November 4, 2024 3:50 PM (20 minutes)

Wide bandgap zirconia attracts considerable attention because of its mechanical, dielectric, thermal and corrosion properties as well as its broad luminescent spectrum. This latter can be tuned by doping with various elements. Doping with yttrium stabilises tetragonal and cubic zirconia structures at room temperature. Simultaneously, zirconia intrinsic luminescence changes because additional oxygen vacancies appear for Y charge compensation. Rare-earth elements introduced in Zr cites demonstrate specific luminescence which is very sensitive to host structure. This feature can be used to recognize the contribution of zirconia polymorphs. Thus, elucidating the interrelation between zirconia structure and intrinsic- and dopant-related luminescence is important. Such a study becomes more attractive when zirconia is codoped with several impurities.

In the present work, the structural and light-emitting properties of undoped, Y-doped and (Y, Eu)co-doped zirconia ceramics sintered at 1100–1600  $^{\circ}$ C were analyzed using Raman scattering, IR reflection spectroscopy, UV-vis diffuse reflection and XRD methods. Luminescence and luminescence excitation spectra were studied using the DESY synchrotron facilities (PETRA III beamline P66) in the 200-900 nm and 120-330 nm spectral ranges, respectively, at helium and room temperatures. The analysis of exciton-emission maps allowed us to separate the contribution of hostrelated and dopant-related luminescence, and to get insight on the luminescence excitation mechanism. Based on the complex characterization, the approach for monitoring zirconia lattice transformation using optical methods was proposed.

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### Type of presence

Presence at Taras Shevchenko National University

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Presenter: Dr KHOMENKOVA, Larysa (V. Lashkaryov Institute of Semiconductor Physics)

**Session Classification:** Advanced Luminescence and Spectroscopy Techniques at DESY: Instruments, Materials, and Applications

Type: Invited Talk

# Establishing the Ukrainian Synchrotron (and Neutron) Community organization

Monday, November 4, 2024 9:00 AM (10 minutes)

Ukrainian synchrotron and neutron users' community (USyNC) is a very young organization that is just taking the first steps towards official registration. Ukrainian synchrotron and neutron radiation users' organization was officially founded at the meeting on November 2, 2023. There are 70-80 active users of synchrotron radiation in Ukraine, based or associated with Ukrainian institutions. At the same time, Ukraine is the most recent country to have got a representation in European synchrotron and neutron users' organization ESUO, with representatives being elected to ESUO at the 19th General Assembly.

This talk presents retrospective and tasks as well as recent activities and achievements of the organization.

### Type of presence

Presence online

Primary author: Dr CHUKOVA, Oksana (Taras Shevchenko National University of Kyiv)

Presenter: Dr CHUKOVA, Oksana (Taras Shevchenko National University of Kyiv)

**Session Classification:** Unifying Efforts: Developing the Ukrainian Synchrotron Community and Research Infrastructure

Type: Invited Talk

# Nonlinear plasmonic nanostructures for quadratic nonlinear optics

Thursday, November 7, 2024 1:00 PM (30 minutes)

We report the quadratic nonlinear optical responses of noble metal nanoparticles with various size and shapes, and their corresponding hyperpolarizability  $\beta$  values as measured via the Harmonic Light Scattering technique at 1.064 µm.

First we investigate the influence of surface area of gold and silver nanospheres and nanorods on their  $\beta$  values, and explore the validity limit of their purely dipolar origin. By studying gold and silver nanorods with different surface areas, we evidence the predominance of these surface effects over shape factors.

Second, we report the synthesis and characterization of platinum "nanoflowers" (PtNFs) with different sizes. These PtNFs display exceptionally strong first hyperpolarisabilities, but particle surface corrugation is shown to govern these huge  $\beta$  values, with a very limited contribution from plasmonic effects.

In a third part, we synthesize and investigate the  $\beta$  values of non-centrosymmetric gold nanoprisms (NPrs). Their  $\beta$ 's not only display a linear dependence with surface area but also strongly depend on the sharpness of NPr corners. Their very high values are assigned mainly to the enhancement of electromagnetic fields due to geometrical effects (sharp extremities). This phenomenon dominates over centrosymmetry breaking. These results open the way to the investigation of various nonlinear noble metal nanopolyhedra families.

### Type of presence

Presence online

**Primary authors:** NGO, Hoang Minh (Laboratoire Lumière, Matière et Interfaces, UMR 8537, Ecole Normale Supérieure Paris-Saclay, CentraleSupélec, CNRS, Université Paris-Saclay, 91190 Gifsur-Yvette, France); ZYSS, Joseph (Laboratoire Lumière, Matière et Interfaces, UMR 8537, Ecole Normale Supérieure Paris-Saclay, CentraleSupélec, CNRS, Université Paris-Saclay, 91190 Gif-sur-Yvette, France); Prof. LEDOUX-RAK, Isabelle (Laboratoire Lumière, Matière et Interfaces, UMR 8537, Ecole Normale Supérieure Paris-Saclay, CentraleSupélec, CNRS, Université Paris-Saclay, 91190 Gif-sur-Yvette, France); Prof. LEDOUX-RAK, Isabelle (Laboratoire Lumière, Matière et Interfaces, UMR 8537, Ecole Normale Supérieure Paris-Saclay, CentraleSupélec, CNRS, Université Paris-Saclay, 91190 Gif-sur-Yvette, France)

**Presenter:** Prof. LEDOUX-RAK, Isabelle (Laboratoire Lumière, Matière et Interfaces, UMR 8537, Ecole Normale Supérieure Paris-Saclay, CentraleSupélec, CNRS, Université Paris-Saclay, 91190 Gif-sur-Yvette, France)

Session Classification: Advances in Nonlinear Optics and Laser-Matter Interactions

Type: Invited Talk

### Tender XAS Beamline at SOLARIS Synchrotron -ASTRA: Overview

Monday, November 4, 2024 11:15 AM (20 minutes)

The ASTRA beamline at the SOLARIS synchrotron (Krakow, Poland) is a relatively new bending magnet beamline, having been open for user operation for just 14 months. As suggested by its name (ASTRA - "Absorption Spectroscopy beamline for Tender energy Range and Above"), it is an X-ray absorption spectroscopy (XAS) beamline. The photon energy range covered by ASTRA extends from 1 to 15 keV, including the tender and part of the hard X-ray energy range. The white beam is monochromatized by a modified Lemonnier type double crystal monochromator (DCM) operating under high vacuum conditions, which can be equipped with different types of crystals to cover the working energy range. XAS spectra are recorded in both transmission and fluorescence modes. The beamline is equipped with an X-ray camera, facilitating precise sample positioning for XAS. Measurements are controlled by the specially developed program AstraLibra, which features a user-friendly interface and advanced functionalities.

ASTRA is a reconfigurable beamline designed to study a wide range of samples within dynamic environments. For example, the beamline enables researchers to investigate microstructural changes that occur during the charging and discharging of batteries, utilizing XANES spectroscopy in transmission mode within both the hard and tender energy ranges. Additionally, ASTRA's users have successfully conducted in-situ experiments in the tender energy range at elevated temperatures with gas flow, providing critical insights into material behaviours under realistic operating conditions. The beamline is equipped with specialized cells designed for measuring samples in liquid phases, making it ideal for both in-situ and operando studies. This capability has been successfully demonstrated, highlighting ASTRA's significant contribution to advancing research in material sciences and related fields.

Moreover, the implementation of a combination of XAS and Raman spectroscopy at the ASTRA beamline is in commissioning. This development will enable researchers to record XAS and Raman spectra simultaneously, providing a possibility for comprehensive material analysis. Once operational, this combined capability will significantly enhance the scope and depth of research that can be conducted, particularly in studying complex processes and materials under operating conditions in the tender energy range. During the presentation, technical aspects of the beamline will be discussed, and selected results of ex-situ and in-situ experiments will be presented.

Acknowledgements: The development of the ASTRA beamline was partly supported within the grant, Innovative Hochschule –Leuchtturm NR - Aus der Höhe in die Breite"(03-IHS-084) by the Federal Ministry of Education and Research, Germany and within the EU Horizon 2020 programme (952148-Sylinda).

### Type of presence

Presence online

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Poland); BRZYSKI, Marcin (National Synchrotron Radiation Centre SOLARIS Jagiellonian University, Kraków, 31-007, Poland); PISZAK, Marcel (National Synchrotron Radiation Centre SOLARIS Jagiellonian University, Kraków, 31-007, Poland); LICHTENBERG, Henning (National Synchrotron Radiation Centre SOLARIS Jagiellonian University, Kraków, 31-007, Poland); Prof. HORMES, Josef (University of Bonn, Bonn, 53113,Germany); Prof. PRANGE, Alexander (Hochschule Niederrhein University of Applied Sciences, Krefeld, 47805, Germany)

**Presenter:** Dr MAXIMENKO, Alexey (National Synchrotron Radiation Centre SOLARIS Jagiellonian University, Kraków, 31-007, Poland)

**Session Classification:** Unifying Efforts: Developing the Ukrainian Synchrotron Community and Research Infrastructure

Type: Oral

### Addressing perovskite stability: crafting an protective layer for sustainable solar cells with the use of synchrotron-based X-ray spectroscopy techniques

Monday, November 4, 2024 5:20 PM (15 minutes)

Our research explores the possibility to enhance the stability and functionality of perovskite solar cells through the encapsulation of these materials with isomorphically substituted calcium hydrox-yapatite (Ca10-zXz(YO4)6(OH)2, where X = Ni, Fe, Cu; Y = V, P) as a transparent encapsulating layer. Building upon recent findings on the electronic structure of calcium apatites, we aim to optimise the composition and properties of the encapsulating layer to suit the requirements of potential photovoltaic applications. This encapsulation approach addresses the key challenges of perovskite degradation due to moisture and oxygen exposure, as well as mitigates the environmental hazard of lead leakage.

The project aims to explore the local environment and structure of the compounds in consideration, in particular the nature of Ca-O, P-O, Fe-O bonds, as well as the Pb-I bond, which is responsible for phase transitions in perovskite and poor stability of solar cells; establish the mechanisms of ion migration in the perovskite structure and study the dynamics of charge transfer. To achieve this, synchrotron-based techniques such as micro-X-ray fluorescence ( $\mu$ XRF), X-ray absorption spectroscopy ( $\mu$ XAS), and X-ray photoelectron spectroscopy will be integrated, in conjunction with theoretical calculations, in order to gain insight into the perovskite-apatite interface. The combination of high-resolution spectroscopic analysis and quantum mechanical modelling allows for precise control over charge dynamics, local atomic structures, and ion migration pathways within the cell.

Furthermore, the project aims to facilitate the development of a dedicated Ukrainian beamline at the SOLARIS synchrotron facility, boosting research infrastructure and expertise in Ukraine.

#### Type of presence

Presence at Taras Shevchenko National University

**Primary author:** Dr KARBIVSKYY, Volodymyr (Kurdyumov Institute for Metal Physics of the NAS of Ukraine)

**Co-authors:** Mr SUKHENKO, Ihor (Kurdyumov Institute for Metal Physics of the NAS of Ukraine); Dr KURGAN, Nataliia (Kurdyumov Institute for Metal Physics of the NAS of Ukraine); Dr SHULYMA, Serhii (Kurdyumov Institute for Metal Physics of the NAS of Ukraine)

Presenter: Mr SUKHENKO, Ihor (Kurdyumov Institute for Metal Physics of the NAS of Ukraine)

Session Classification: X-ray Microscopy and Spectroscopy of Functional Material

Type: Oral

### Vacuum ultraviolet time-resolved luminescence at P66 at DESY: instrument characteristics and applications

Monday, November 4, 2024 3:30 PM (20 minutes)

In October 2024, P66 vacuum ultraviolet (VUV) time-resolved luminescence beamline marks three years of successful operation. Inheriting its main features from previous SUPERLUMI beamline at DORIS III storage ring [1], P66 is requested by leading scientists from more than 30 scientific groups around the world. Excitation and emission energy scans of the luminescence intensity within a unique excitation range of 3.7-40 eV, enabled by the ultrahigh vacuum conditions and added the time resolution down to circa 150 ps, employing the pulsed nature of the synchrotron radiation at DESY and fast detectors and electronics, make the setup a singular instrument to probe impurity/defect states, to determine the bandgap of dielectric materials and to unravel the energy relaxation and recombination mechanisms after VUV excitation. Absorbed by nearly all materials, VUV is a universal tool to study matter, in particular surfaces (the penetration depth of this radiation is circa 100 nm). An integrated cryostat provides a possibility to cool samples down to 8 K with the use of liquid helium, so even the weakest luminescence is enhanced, cutting away thermal relaxation processes. The applications of the method range from material science to fundamental physics: from fast scintillators for medical imaging and LEDs [2] to persistent phosphors for safety signs and luminophores for colour display panels are studied next to the first principles spectroscopy of nanophosphors [3].

References:

- 1. Zimmerer, G., SUPERLUMI: A unique setup for luminescence spectroscopy with synchrotron radiation. Rad. Meas, 42, 2007, 4-5, p. 859-864.
- 2. Jary, V. et al., Efficient Ultrafast Scintillation of KLuS2: Pr3+ Phosphor: A Candidate for Fast-Timing Applications. Phys. Rev. Applied, 19, 2023, 034092.
- 3. Pankratov, V. et al., Luminescence and Vacuum Ultraviolet Excitation Spectroscopy of Nanophosphors under Synchrotron Irradiation. Phys. Status Solidi B, 259, 2022, 2100475.

### Type of presence

Presence online

**Primary authors:** Mr KATAEV, Aleksandr (Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, Hamburg 22607, Germany); Dr KOTLOV, Aleksei (Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, Hamburg 22607, Germany); CHUKOVA, Oksana (Taras Shevchenko National University of Kyiv); Dr SMORTSOVA, Yevheniia (Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, Hamburg 22607, Germany)

**Presenter:** Dr SMORTSOVA, Yevheniia (Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, Hamburg 22607, Germany)

**Session Classification:** Advanced Luminescence and Spectroscopy Techniques at DESY: Instruments, Materials, and Applications

25TH SYMPOSI ··· / Report of Contributions

Vacuum ultraviolet time-resolved  $\cdots$ 

Type: Invited Talk

# **Challenges to Carbon Neutrality**

*Tuesday, November 5, 2024 8:15 AM (40 minutes)* 

In 2023, the global average temperature got 1.52degC higher than that of pre-industrial time, already exceeding the +1.5degC limit set by IPCC. There won't be any winner in the fight against global climate change. If we are unable to cooperate now, we will all fall down, going into the future of catastrophic starvation, water and energy shortage, plague, anything horrible you can imagine.

Our kind of people like to talk about new technologies for clean energy, energy saving and storage ...but we must remember that these "green techs" are simply used for winning in the economic competition, rather than helping each other. For example, extreme exploitation and human rights abuse are taking place in Congo Republic, for cobalt mining, that is essential for lithium batteries. People are also seeking precious minerals deep in ocean, where they still know almost nothing about its ecosystem. Recent study found that those nodules of precious metals are acting like batteries for water electrolysis to supply oxygen to the aerobic lives in the deep sea. Test mining of the nodules thus resulted in complete extinction of the lives, as they were dependent on this non-photosynthetic oxygen!

Technological development could reduce GHG emission per USD of GDP to 1/3 in 100 years, while global GDP increased more than 8 times in the last 60 years. It is obvious that technological advancement cannot solve the problem, but every one of us will have to learn a new way of life. Geographical and historical background of development results in different habits and mindset when talking about sustainable society. The USA has 333 million people, No. 1 GDP of 27 trillion USD, self-sufficient for food and energy, whereas Japan has 125 million people, No. 4 GDP of 4.2 trillion USD, 90% of energy and 60% of food are imported. "Global economy" is the word for Japan. Global supply chain is the lifeline for Japanese, but majority of people living on that island, enjoying its slow and comfortable life, are unaware of this. I would like to share some of my thoughts about the importance of international collaboration for co-existence.

### Type of presence

Presence online

**Primary author:** Prof. YOSHIDA, Tsukasa (Graduate School of Organic Materials Science, Yamagata University)

**Presenter:** Prof. YOSHIDA, Tsukasa (Graduate School of Organic Materials Science, Yamagata University)

Session Classification: Workshop on Sustainable Materials and Technologies

Track Classification: Workshop on Sustainable Materials and Technologies

Type: Oral

# Inverse design of antireflection silicon-on-silicon coatings

Thursday, November 7, 2024 4:30 PM (15 minutes)

Designer gratings, also known as metagratings, can be tuned to preform various kinds of tasks, such as amplify deflection in a particular diffraction order, increase or decrease transmission and reflection [1]. A typical task for various kinds of coatings is to reduce reflection from a surface. Inspired by this, we set out to design a single-layer silicon metagrating as an antireflection cover for solar cells, itself made from silicon, which introduces high reflection of light (30-50%) from a flat interface, a significant inefficiency in the cells' ability to capture incident radiation [2]. To achieve desired low reflection (around 5% or less) for both polarizations, a range of incidence angles and a wide band from 400 to 1200 nm, a large space of unit cell designs of the periodic structure has to be explored. In this work, we apply an inverse design approach [3] to solve this task and denerate patterns which demonstrate the required performance.

- 1. Quaranta G., Basset G., Martin O. J., Gallinet B. Recent advances in resonant waveguide gratings // Las. Photonics Rev. –2018. –12. –№9. –P. 1800017.
- 2. Mascaretti L. et al. Designing metasurfaces for efficient solar energy conversion // ACS Photonics. -2023. -10. -№12. -P. 4079.
- 3. Jiang J., Fan J. A. Multiobjective and categorical global optimization of photonic structures based on ResNet generative neural networks // Nanophotonics. –2020. –10. –№1. –P. 361.

### Type of presence

Presence online

Primary author: OVCHARENKO, Anton (V. N. Karazin Kharkiv National University)

**Co-author:** YERMAKOV, Oleh (V.N. Karazin Kharkiv National University, 4 Svobody Square, Kharkiv 61022, Ukraine)

Presenter: OVCHARENKO, Anton (V. N. Karazin Kharkiv National University)

Session Classification: Advances in Metasurfaces and Plasmonic Nanostructures

Type: Invited Talk

# SOLARIS Centre - facility status and research highlights

*Monday, November 4, 2024 10:35 AM (20 minutes)* 

The SOLARIS synchrotron in Krakow, Poland, is a third-generation light source operating at 1.5 GeV electron energy. The project was officially initiated in 2010, the first synchrotron light was observed in 2016, and the first user experiment was performed in 2018. At present, SOLARIS Centre offer access to 10 research instruments at seven beamlines and two cryo-electron microscopes, and is constructing five additional end-stations. Research opportunities offered by SOLARIS, the only synchrotron in Central-Eastern Europe, allow for conducting unique scientific projects in fundamental research and applied sciences. Access to the research infrastructure of SOLARIS Centre is free of charge and provided upon the assessment of beamtime proposals by the international review panel. Financial support to foreign user visits, including Ukrainian researchers, is possible through several schemes, e.g. Horizon Europe projects NEPHEWS and RIANA as well as CERIC-ERIC consortium.

### Type of presence

Presence online

**Primary author:** Prof. SIKORA, Marcin (SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, Czerwone Maki 98, 30-392 Krakow, Poland)

**Presenter:** Prof. SIKORA, Marcin (SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, Czerwone Maki 98, 30-392 Krakow, Poland)

**Session Classification:** Unifying Efforts: Developing the Ukrainian Synchrotron Community and Research Infrastructure

Type: Invited Talk

### Analytical model for the switching voltage and gain coefficient of a CMOS inverter with nanochannel 2D transistors

*Thursday, November 7, 2024 9:15 AM (45 minutes)* 

The study presents an analytical model for the switching voltage and gain factor of a CMOS inverter with 2D nanochannel transistors. The derived expressions enable the modeling of these two fundamental parameters of the device, which serves as the foundation for logic elements in contemporary nanoelectronics. The feasibility of creating efficient inverters with a high gain factor based on transistors with channels made of 2D monolayers of transition metal dichalcogenides and arrays of carbon nanotubes has been confirmed. It was demonstrated that the gain factor is restricted by the drain induced barrier lowering (DIBL) effect, which is undesirable for FETs (when DIBL trends to zero the gain factor becomes infinitely large).

#### Type of presence

Presence online

**Primary authors:** Prof. STRIKHA, Maksym (Taras Shevchenko National University of Kyiv, Faculty of Radiophysics, Electronics and Computer Systems, 4g Glushkov Avenue, Kyiv, Ukraine); Mr HURIEIEV, M. (Taras Shevchenko National University of Kyiv, Faculty of Radiophysics, Electronics and Computer Systems, 4g Glushkov Avenue, Kyiv, Ukraine)

**Presenter:** Prof. STRIKHA, Maksym (Taras Shevchenko National University of Kyiv, Faculty of Radiophysics, Electronics and Computer Systems, 4g Glushkov Avenue, Kyiv, Ukraine)

Session Classification: Optics and High Technology Material Science: Plenary

Advancing Ukrainian Science: T

Contribution ID: 107

Type: Invited Talk

# Advancing Ukrainian Science: The Micro/Nano XAS Beamline at SOLARIS Under the 'Light for Ukraine' Initiative

Monday, November 4, 2024 10:15 AM (20 minutes)

Type of presence

Presence online

Primary author: Prof. PATTHEY, Luc (PSI - Paul Scherrer Institut)

Presenter: Prof. PATTHEY, Luc (PSI - Paul Scherrer Institut)

**Session Classification:** Unifying Efforts: Developing the Ukrainian Synchrotron Community and Research Infrastructure

Track Classification: USyNC Workshop

Dichroic Ptychography in the Soft …

Contribution ID: 108

Type: Invited Talk

# Dichroic Ptychography in the Soft X-ray Energy Regime

Monday, November 4, 2024 4:30 PM (30 minutes)

Type of presence

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Presence online

**Primary author:** Dr BUTCHER, Tim A. (Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, 12489 Berlin, Germany)

**Presenter:** Dr BUTCHER, Tim A. (Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, 12489 Berlin, Germany)

Session Classification: X-ray Microscopy and Spectroscopy of Functional Material

Track Classification: USyNC Workshop

Type: Poster

# Optical thermometry: fluorescence of rear-earth ions in aluminum nitride thin films

Friday, November 8, 2024 5:22 PM (3 minutes)

Non-contact optical thermometry is based on temperature dependence of fluorescence intensity ratio (FIR) of two spectral lines. Recently, fluorescence of rear-earth ions incorporated in wide-gap materials has been widely used for accurate temperature sensing.

Eu-doped and Sm-doped AlN thin films prepared by radio frequency magnetron sputtering were studied in terms of their applicability as temperature sensors.

In Eu-doped film both trivalent Eu3+ and divalent Eu2+ ions were detected. The film emitted intense red light under UV excitation, where narrow intense lines from the excited level 5D0 of Eu3+ dominated in the spectra. Eu2+ manifested itself as a low-intense fluorescence band at 430–570 nm. The fluorescence excitation spectra allowed to conclude the Eu excitation by nonradiative energy transfer. The temperature dependence of the thermally coupled levels 5D1 and 5D0 of Eu3+ ions was studied in detail from -160 to +250 C. The levels showed an absolute sensitivity up to 0.003 K–1. Approaching a broadband multi-peak detection and the FIR of Eu2+/Eu3+, a much higher sensitivity up to 0.01 K–1 was achieved.

The Sm-doped film emitted a bright orange-red light under UV excitation. The most intense bunches at 580, 621 and 660 nm were identified as due to radiative transitions from the excited Sm3+ level 4G5/2 to the ground ones 6H5/2, 6H7/2 and 6H9/2, respectively. Considering ratios between integral intensities of the Sm3+ line bunches in the mentioned range, the maximum absolute and relative sensitivities of ~1.3x10-3 and 1.9x10-3 K-1 were obtained, respectively.

### Type of presence

Presence online

**Primary authors:** Dr LI, Baikui (College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen, China); Dr PENG, Dengfeng (College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen, China); Dr ZHANG, Feihong (College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen, China); Dr WU, Honglei (College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen, China); Dr LUO, Jiangcheng (College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen, China); Dr LUO, Jiangcheng (College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen, China); Dr JIN, Lei (College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen, China); Dr DATSENKO, Oleksandr (Taras Shevchenko National University of Kyiv, Faculty of Physics); Dr WANG, Peiyao (College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen, China); GOLOVYNSKYI, Sergii (College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen, China); Dr SUN, Zhenhua (College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen, China); Dr WANG, Zhiyuan (College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen, China); Dr WANG, Zhiyuan (College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen, China); Dr WANG, Zhiyuan (College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen, China); Dr WANG, Zhiyuan (College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen, China); Dr WANG, Zhiyuan (College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen, China)

**Presenter:** KRAVCHENKO, Vladyslav (Taras Shevchenko National University of Kyiv, Faculty of Physics)

25TH SYMPOSI ··· / Report of Contributions

Optical thermometry: fluorescen  $\cdots$ 

### Session Classification: Poster Session

Towards control of femtosecond l  $\cdots$ 

Contribution ID: 110

Type: Oral

# Towards control of femtosecond laser structuring of silicon

Wednesday, November 6, 2024 8:45 AM (20 minutes)

To be complited soon

### Type of presence

Presence at Taras Shevchenko National University

**Primary authors:** DMYTRUK, Andriy (Institute of Physics NASU); Dr KARLASH, Anna; Prof. DMYTRUK, Igor; Prof. BLONSKYI, Ivan; Prof. BONDAR, Mykhaylo; Dr BEREZOVSKA, Natalia; Dr KADAN, Viktor; Mr HRABOVSKYI, Yevhen

**Presenter:** DMYTRUK, Andriy (Institute of Physics NASU)

Impact of sulfur vacancies on the ···

Contribution ID: 111

Type: Invited Talk

# Impact of sulfur vacancies on the light emission and transport properties of MoS2 structures

Tuesday, November 5, 2024 1:00 PM (20 minutes)

In the last decade, the rise of monolayer (ML) transition metal dichalcogenides (TMDs) has changed the paradigm for the coupling of two-dimensional materials to a well-established platform without the constraints imposed by epitaxies such as crystal-lattice match or chemistry compatibility. The employment of semiconducting monolayers has resulted in several applications in different fields such as electronics, valleytronics, energy storage, photovoltaics, light detection and chemical sensing.

Among TMDs, molybdenum disulfide (MoS2) has been demonstrated to be the most versatile material for optoelectronic and photonic applications due to its layer-dependent optical properties. In the monolayer regime, MoS2 exhibits a direct optical bandgap in the visible range, which makes it a good candidate for novel applications ranging from photonics to optoelectronics.

In this work, we highlight the impact of sulfur vacancies in two complete different MoS2 based systems:

 we univocally demonstrate the role of sulfur vacancies in mechanically exfoliated multilayer flakes for the engineering of infrared light emissions, with possible applications in Telecom/Datacom.
 we report the unexpected electron transport suppression in monolayer MoS2 encapsulated graphene field-effect transistor, caused by the presence of sulfur vacancies in the MoS2 monolayer.

#### Type of presence

Presence online

Primary author: Dr FABBRI, Filippo (NANO CNR)

Presenter: Dr FABBRI, Filippo (NANO CNR)

Session Classification: Workshop on Sustainable Materials and Technologies

Micro-XRD Imaging of Lattice C ...

Contribution ID: 112

Type: Oral

# Micro-XRD Imaging of Lattice Contraction Induced by Resistive Switching in Chromium-Doped V<sub>2</sub>O<sub>3</sub> Mott Insulator

Monday, November 4, 2024 5:00 PM (20 minutes)

Type of presence

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Presence online

Primary author: Dr BABICH, Danylo (PSI - Paul Scherrer Institut)

Presenter: Dr BABICH, Danylo (PSI - Paul Scherrer Institut)

Session Classification: X-ray Microscopy and Spectroscopy of Functional Material

Track Classification: USyNC Workshop

Type: Invited Talk

# **Attosecond X-ray Free-Electron Lasers**

Monday, November 4, 2024 1:00 PM (30 minutes)

'Seeing means believing'as the old axiom says. Every year around 50 000 scientists worldwide use X-ray photon beams at synchrotron and X-ray Free-Electron Laser (XFEL) facilities to image the structure and motion of matter. X-ray studies on protein crystallography and X-ray driven catalysis in biomolecules became reality with the development of synchrotron light sources. The advert of XFELs has enabled biological imaging with femtosecond X-ray pulses, which is nowadays a key instrument for structural biology. Recently, attosecond lasing was demonstrated at several XFELs and first user experiments on charge migration and photoionization started. In this talk, I will discuss the present state-of-the-art of ultrashort pulse generation in XFELs and review some recent technological developments.

### Type of presence

Presence online

**Primary author:** Prof. GORYASHKO, Vitaliy (Uppsala University, Sweden; RIKEN, SPring-8, Japan)

Presenter: Prof. GORYASHKO, Vitaliy (Uppsala University, Sweden; RIKEN, SPring-8, Japan)

**Session Classification:** Exploring Ultrafast Phenomena with the XFEL: Instruments, Capabilities, and Applications

Track Classification: USyNC Workshop

High-throughout compositional s ...

Contribution ID: 114

Type: Invited Talk

# High-throughout compositional screening of new sustainable (green) perovskite materials for energy conversion (light harvesting and emission)

Tuesday, November 5, 2024 9:30 AM (30 minutes)

Type of presence

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Presence online

**Primary author:** Dr STROYUK, Oleksandr (Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (HI ERN), Germany)

**Presenter:** Dr STROYUK, Oleksandr (Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (HI ERN), Germany)

Session Classification: Workshop on Sustainable Materials and Technologies

Type: Invited Talk

## Facts and Artifacts in Optical and Structural Characterization of Emerging Materials for Renewable and Sustainable Energy

*Tuesday, November 5, 2024 4:50 PM (20 minutes)* 

The p-type emerging materials for photovoltaics such as inorganic chalcogenides and organohalide perovskites or other materials for renewable and sustainable energy applications in thin film or powder form are often reported with misleading/wrong optical and structural parameters. Thus, the credibility and significance of many published works should be questioned by the readers. Following a smart documentation by note taking including mind mapping, any should create an integrated protocol to find out the truth.

First issue concerns the XRD analysis. Several pathways will be given to identify correctly the crystalline phase, the lattice parameters, to find out and to prove the existence or absence of secondary phases and to determine the average crystallite sizes.

Second problem regards optical measurements and methods to extract the band gap. Can at least qualitatively observe the band gap difference within a samples batch? Is considered the possible differences between surfaces of the films and their bulk? Examples on inorganic chalcogenides and on organohalide perovskites will be given.

Also, tips and tricks concerning complementary techniques such as Raman spectroscopy and Xray photoelectron spectroscopy will be revealed, needed to sustain the conclusions or, why not, to change even the initial scientific findings.

The authors acknowledge the financial support from the Romanian Ministry of Research, Innovation and Digitalization and UEFISCDI in the framework of PC3-PN23080303, PN-III-P4-ID-PCE-2020-0827 and ERANET-M-3-ERANET-Lightcell projects.

### Type of presence

Presence online

#### Primary author: Dr GALCA, Aurelian Catalin (National Institute of Materials Physics)

**Co-authors:** Mr TOMULESCU, Andrei Gabriel (National Institute of Materials Physics); Dr BESLEAGA, Cristina (National Institute of Materials Physics); Dr PINTILIE, Ioana (National Institute of Materials Physics); Dr LEONAT, Lucia Nicoleta (National Institute of Materials Physics); Dr EL KHOUJA, Outman (National Institute of Materials Physics); Dr DERBALI, Sarah (National Institute of Materials Physics); Dr STANCU, Viorica (National Institute of Materials Physics)

Presenter: Dr GALCA, Aurelian Catalin (National Institute of Materials Physics)

Session Classification: Workshop on Sustainable Materials and Technologies

Type: Invited Talk

## **OPTICA: Navigating Emerging Opportunities in Optics and Photonics**

Thursday, November 7, 2024 10:00 AM (30 minutes)

Yann Amouroux represents Optica, the international society dedicated to advancing Optics and Photonics Worldwide.

In this non-technical talk, he will discuss career development, how learned societies encourage international collaboration, and some of the emerging trends in optics and photonics.

The world is changing rapidly, with constant challenges taking place; what are the opportunities for early career researchers, and what are the prospects for fresh graduates?

Type of presence

Primary author: Mr AMOUROUX, Yann (Director, Europe, OPTICA)

Presenter: Mr AMOUROUX, Yann (Director, Europe, OPTICA)

**Session Classification:** Professional Development in Optics: Navigating Opportunities and Entrepreneurship

The European Synchrotron and F  $\,\cdots\,$ 

Contribution ID: 117

Type: Invited Talk

# The European Synchrotron and FEL User Organisation (ESUO)

Monday, November 4, 2024 9:35 AM (15 minutes)

Type of presence

Presence online

Primary author: Prof. MCGUINNESS, Cormac (ESUO / Trinity College Dublin)

Presenter: Prof. MCGUINNESS, Cormac (ESUO / Trinity College Dublin)

**Session Classification:** Unifying Efforts: Developing the Ukrainian Synchrotron Community and Research Infrastructure

Track Classification: USyNC Workshop

NEPHEWS support for Ukrainian ···

Contribution ID: 118

Type: Invited Talk

# NEPHEWS support for Ukrainian User communities use of Neutron and Photon sources

Monday, November 4, 2024 9:50 AM (15 minutes)

Type of presence

Presence online

**Presenter:** Mr PIWOWARCZYK, Piotr (SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, Czerwone Maki 98, 30-392 Krakow, Poland)

**Session Classification:** Unifying Efforts: Developing the Ukrainian Synchrotron Community and Research Infrastructure

Track Classification: USyNC Workshop

Type: Oral

### Tailoring MoS<sub>2</sub> Optical Response: A Plasmonic Nanoparticle Approach

Tuesday, November 5, 2024 2:00 PM (15 minutes)

Two-dimensional (2D) materials like  $MoS_2$  hold immense promise for novel optoelectronic and nanophotonic applications. However, their practical implementation is often hindered by limited photoluminescence and Raman efficiencies. Plasmonic enhancement using metal nanoparticles provides an effective approach to overcome these limitations by enhancing light-matter interactions in these materials. In this work, we investigate the impact of plasmonic nanostructures, specifically silver (Ag) and gold (Au) nanoparticles of varying geometries, on the Raman and PL spectra of monolayer and few-layer  $MoS_2$ . Nanotriangles, nanorods, and nanospheres of Ag and Au are used to explore the effect of shape, size, and plasmonic properties on the enhancement factor.

Our findings reveal a significant enhancement in both Raman and PL intensities. Notably, nanotriangles and nanorods exhibit the most pronounced enhancement, attributed to the generation of intense plasmonic hot spots at their sharp edges and tips. The enhancement factors achieved for Raman and PL spectra were up to 6.8 times for silver nanotriangles and 4.3 times for gold nanorods, respectively. These enhancements are attributed to plasmonic coupling and the generation of hot spots that amplify the electric field in the vicinity of  $MoS_2$  flakes. Additionally, the increased PL intensity is also linked to the injection of hot electrons from metal nanostructures, facilitating exciton generation and improving emission efficiency.

This study underscores the crucial role of nanoparticle geometry in optimizing plasmonic enhancement in 2D materials, providing valuable insights into the intricate physical mechanisms governing light-matter coupling within hybrid nanostructures. These findings are highly promising for the development of next-generation optoelectronic and photonic devices, including photodetectors, sensors, and other advanced technologies.

### Type of presence

Presence online

**Primary authors:** Ms IRFAN, Iqra (Shenzhen University); Mr SERGII, Golovynskyi (Shenzhen University)

Presenter: Ms IRFAN, Iqra (Shenzhen University)

Session Classification: Workshop on Sustainable Materials and Technologies

Type: Oral

### Laser Absorption Spectroscopy of Electric Discharge Plasma with Copper Vapour Admixtures

Friday, November 8, 2024 3:45 PM (15 minutes)

The spatial distribution of number density of copper atoms in the plasma of electric arc discharge with copper vapour admixtures is determined by method of linear laser absorption spectroscopy. For this purpose, the discharge gap is illuminated by radiation of laser on the copper vapours. The absorption coefficient and, therefore, number density of absorbing species is determined from the experimentally obtained optical thickness of plasma.

The investigation of spatial distribution of optical thickness of plasma with copper vapour admixtures is carried out by the experimental setup using the laser on copper vapours "Kriostat 1"as a radiation source. The generation spectrum of this laser type contains two Cu I spectral lines: 510.5 and 578.2 nm. The diffraction grating is additionally used in optical scheme to separate one of these spectral lines.

The use of a two-dimensional CMOS matrix as a registration device provides possibilities to study the spatial distribution of number density of copper atoms in the plasma of electric discharges with copper vapour admixtures. The discharge gap was probed by laser radiation beam on the wave-length, separated by the diffraction grating. The registration of the beam which passed through the plasma is performed in the experiments by the matrix of 6000x4000 pixels. The recorded digital image is treated by the specially developed software. Thus, the proposed technique principally enables to obtain simultaneously the 2D distribution of plasma optical thickness. ACKNOWLEDGMENT

This work was supported by the National Research Foundation of Ukraine (Grant № 167/0169)

### Type of presence

Presence at Taras Shevchenko National University

**Primary author:** Ms SYCH, Daryna (Faculty of Radiophysics, Electronics and Computer Systems of Taras Shevchenko National University of Kyiv)

**Co-authors:** MURMANTSEV, Aleksandr (Faculty of Radiophysics, Electronics and Computer Systems of Taras Shevchenko National University of Kyiv); Dr IVANISIK, Anatoliy (Faculty of Radiophysics, Electronics and Computer Systems of Taras Shevchenko National University of Kyiv); Prof. VEKLICH, Anatoly (Faculty of Radiophysics, Electronics and Computer Systems of Taras Shevchenko National University of Kyiv)

**Presenter:** Ms SYCH, Daryna (Faculty of Radiophysics, Electronics and Computer Systems of Taras Shevchenko National University of Kyiv)

Session Classification: Laser-Plasma Interactions and Spectroscopy

Type: Invited Talk

# Physics and modeling of quantum dot solar cells

Tuesday, November 5, 2024 2:40 PM (20 minutes)

The idea of using quantum dots (QD) to extend the spectral sensitivity and improve the efficiency of solar cells was first put forward by Aroutiounian et al. (J. Appl. Phys. 89, 2268, 2001). QDs indeed provide several useful knobs in photovoltaics, such as tuning the bandgap for a certain spectrum and concentration, realizing current-matched multiple junction cells, and improving radiation hardness in space. On the other hand, the expectation of overcoming the Shockley-Queisser limit of single-gap cells with QD solar cells is yet unfulfilled. For this to happen, it is necessary to engineer the nanostructures to suppress phonon assisted coupling between extended and quantum-confined states, and within intraband confined states too. In this way, one could realize by means of QDs the intermediate band (IB) solar cell (Luque et al., Phys. Rev. Lett., 78, 26, 1997), which has a theoretical efficiency about 50% higher than its single-gap counterpart under unconcentrated light. Three decades of extensive research, mostly on self-assembled III-V QDs, has led to observe the fundamental mechanisms of the IB solar cell at cryogenic temperatures but the demonstration of a high efficiency IB cell is yet to come. Recently, new materials have emerged, such as strain-free III-V QDs and colloidal QDs into perovskite absorbers, with promising features for IB operation at room temperature. In this talk, I will revisit the physics and limits of QD solar cells, considering optical and transport simulations and discuss possible ways forward for their development, both in the perspective of single-gap and IB operation.

### Type of presence

Presence online

**Primary author:** Prof. CAPPELLUTI, Federica (Department of Electronics and Telecommunications, Politecnico di Torino, ITALY)

**Presenter:** Prof. CAPPELLUTI, Federica (Department of Electronics and Telecommunications, Politecnico di Torino, ITALY)

Session Classification: Workshop on Sustainable Materials and Technologies

Type: Poster

### IMPEDANCE SPECTROSCOPY OF GeSn/Ge/Si STRUCTURES AT DIFFERENT TEMPERATURES

Friday, November 8, 2024 4:45 PM (3 minutes)

Structures with GeSn films of different thicknesses CVD-grown on Ge/Si substrates were studied by temperature-dependent spectroscopy of impedance Z = Z1 + iZ2 within 1 - 1000 kHz. At lower temperatures, the films revealed insets of the photosensitivity characteristic for interband excitation of GeSn, Ge (direct bandgap) and Si. From the frequency dependencies of real Z1 and imaginary Z2 parts of the impedance, the conductances and carrier relaxation times of the structures at temperatures from 80 to 300 K were extracted. The structures with GeSn films are found to have low-temperature conductivities two order higher and, respectively, relaxation times two order faster than the reference substrate Ge/Si (without GeSn), which reveals an ordinary semiconductor-like temperature dependence of conductance slowly rising at lower temperatures and highly increasing above ~200 K following  $\sim \exp[-E/(kT)]$  with the activation energy E of ~350 meV, which is close to the half of Ge bandgap near 0 K. Contrarywise, the dependences for the GeSn/Ge/Si structures are non-monotonous, passing a minimum at higher temperatures, which is attributed to higher (metal-like) GeSn conductivity. The impedance measurements under illumination within the Si interband excitation show that the photoconductivity versus temperature has a peak at the range of the dark conductance minimum. The data are explained within the ideas of the conductivity of multilayered structures.

This work was supported by the National Research Foundation of Ukraine (2023.03/0060).

#### Type of presence

Presence at Taras Shevchenko National University

**Primary authors:** Mr POCHERPAILO, Andrii; Mr USTINOV, Dmytro; Mr BOZHKO, Oleg; Dr DATSENKO, Oleksandr; Mr KOVANZHI, Petro; KONDRATENKO, Serhiy

**Presenter:** KONDRATENKO, Serhiy

Session Classification: Poster Session

Type: Oral

# Tuneable Excitonic Luminescence in 2D hybrid perovskites

Tuesday, November 5, 2024 10:00 AM (15 minutes)

Two-dimensional hybrid perovskites have attracted considerable interest for combining Van der Waals properties like quantum confinement and reduced dielectric screening with the structural tunability of perovskites. In these materials, both layer composition and sublayer number can be varied, impacting quantum confinement effects. These structures are often modeled as periodic quantum wells separated by transparent organic layers. Here, we show that excitonic luminescence in these quantum wells—specifically peak position, full width at half maximum, and intensity—depends strongly on nanosheet layer count, challenging the assumption of minimal impact from layer number.

Using single crystals of n-butylammonium lead iodide (BAPI) 2D perovskite, micromechanically exfoliated to create nanosheets of differing thickness, we applied atomic force microscopy (AFM), and time-resolved and steady-state photoluminescence microscopy at room and cryogenic temperatures. Variations in excitonic photoluminescence were notable, especially at low temperatures below the order-disorder phase transition, where layer number shifted excitonic PL peaks by up to 120 meV.

#### Type of presence

Presence online

Primary author: Mr SHCHERBAKOV, Andrii (PCI University of Heidelberg)

**Co-authors:** Mr KORTE, Darwin; Dr LIU, Shangpu; Mr W. HEINDL, Markus; Ms SOLTALAB, Nasrin; Dr BODNAR, Stanislav; Mr ZERHOCH, Jonathan; Prof. DESCHLER, Felix

**Presenter:** Mr SHCHERBAKOV, Andrii (PCI University of Heidelberg)

Session Classification: Workshop on Sustainable Materials and Technologies

Type: Oral

# "Green" Aqueous Synthesis, Structural and Optical Properties of Quaternary Cu<sub>2</sub>ZnSnS<sub>4</sub> and Cu<sub>2</sub>NiSnS<sub>4</sub> Nanocrystals

*Tuesday, November 5, 2024 3:20 PM (15 minutes)* 

Elemental substitution in Cu<sub>2</sub>ZnSnS<sub>4</sub>-like chalcogenides opens up the potential to create alternative low-cost photovoltaic and thermoelectric materials with tunable properties. The method of "green" synthesis in aqueous solutions, based on the protocol previously proposed for CZTS [1], has been used to obtain Cu<sub>2</sub>NiSnS<sub>4</sub> (CNTS) nanocrystals (NC). This method opens up possibilities for non-toxic, economical large-scale production.

The structural and optical properties of CXTS NCs (X = Ni, Zn) NCs were studied in colloidal solutions and thin films. Thin films of NCs were deposited on glass substrates by spin coating method. From X-ray diffraction (XRD) and Raman spectroscopy data, it was concluded that the synthesised NCs of CZTS and CNTS with sizes in the range of 1.5 to 2.5 nm are likely to have a kesterite structure with disordered cations. CNTS shows broader diffraction and Raman peaks, indicating a higher degree of cationic disorder than in CZTS. The theoretical calculation of Raman peaks was carried out using the tight binding method to better understand the effect of cationic disorder on Raman spectra. The calculations qualitatively agree with the experimental results. CZTS and CNTS films between 40 and 150 nm thick were prepared from colloidal solutions demonstrating the versatility of the material and its compatibility with thin film deposition techniques. The thickness of the thin films was determined from atomic force microscopy (AFM) and spectroscopic ellipsometry (SE) data. AFM height profiles of low aggregated NCs show an average size in line with XRD analysis. Optical absorption studies of NCs reveal a continuous spectrum in the visible range with a bandgap of approximately  $2.2 \pm 0.3$  eV for both materials positioning them as effective absorbers for solar cell applications. Absorption coefficients for both exceed 10<sup>2</sup> cm<sup>-1</sup> at 700 nm and reach over 10<sup>4</sup> cm<sup>-1</sup> at 400 nm indicating significant light-absorbing capabilities of the material.

These properties highlight the versatility of CNTS and demonstrate the advantages of "green" synthesis methods for the development of sustainable, low-cost nanomaterials for energy applications.[2]

### Type of presence

**Primary author:** Ms IVAKHNO-TSEHELNYK, Oleksandra (Semiconductor Physics & Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology)

**Co-authors:** Dr SELYSHCHEV, Oleksandr (Semiconductor Physics & Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology.); Prof. KONDRATENKO, Serhiy (Taras Shevchenko National University of Kyiv); Prof. DZHAGAN, Volodymyr (Lashkaryov Institute of Semiconductor Physics (ISP), NAS of Ukraine); HERTLING, Lukas (Semiconductor Physics & Research Center for Materials, Architectures and Integration of Nanomembranes

(MAIN), Chemnitz University of Technology); Prof. RT ZAHN, Dietrich (Semiconductor Physics & Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology)

**Presenter:** Ms IVAKHNO-TSEHELNYK, Oleksandra (Semiconductor Physics & Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology)

Session Classification: Workshop on Sustainable Materials and Technologies

Type: Invited Talk

### Low dimensional perovskites for quantum optics and polaritonics

Tuesday, November 5, 2024 11:20 AM (20 minutes)

Metal halide perovskites (MHPs) have become attractive materials for light-matter interaction, and particularly for quantum optic devices [1]. Their advantages include straightforward fabrication by chemical synthesis, a broad bandgap tunability with the composition, the high emission efficiencies, and the high excitonic binding energy. Consequently, low dimensional MHPs have been incorporated in different microcavities resonators to demonstrate lasing, and more recently polariton condensation in cavity coupled lattices [1]. In this direction, perovskites 0D nanocrystals (NCs) and two-dimensional (2D) perovskites have emerged as a low dimensional MHPs with excellent properties to study Jaynes–Cummings or dressed Boson Hamiltonians. In contrast to 3D perovskites, the semiconducting inorganic layer in 2D perovskites passivated with insulating long organic cations forming a 2D quantum well structure owning a higher defect tolerance and resistance against environmental conditions [3]. Here, it will be summarized recent results from the optical characterization of low dimensional MHPs, for low-cost single photon emitters and for high tunability QED approaches, with fibre-based open-access optical microcavities. The open-cavity approach results as an outstanding scheme for the development of the exciting field of quantum polaritonics [4].

[1] M. Esmann, S. C. Wein, C. Antón-Solanas, Solid-State Single-Photon Sources: Recent Advances for Novel Quantum Materials. Adv. Funct. Mater. 2024, 2315936.

[2] Su, R., Ghosh, S., Wang, J. et al. Observation of exciton polariton condensation in a perovskite lattice at room temperature. Nat. Phys. 16, 301–306 (2020)

[3] Setatira Gorji et al. Origin of discrete donor–acceptor pair transitions in 2D Ruddlesden–Popper perovskites. Appl. Phys. Rev. 1 June 2024; 11 (2): 021401

[4] Muñoz-Matutano, G., Wood, A., Johnsson, M. et al. Emergence of quantum correlations from interacting fibre-cavity polaritons. Nature Mater 18, 213–218 (2019) & Delteil, A., Fink, T., Schade, A. et al. Towards polariton blockade of confined exciton–polaritons. Nature Mater 18, 219–222 (2019)

### Type of presence

**Presenter:** Dr MUNOZ MATUTANO, Guillermo (Institut de Ciència dels Materials (ICMUV), Universitat de València. Catedrático José Beltrán 2, 46980 Paterna, Valencia, Spain.)

Session Classification: Workshop on Sustainable Materials and Technologies

25TH SYMPOSI ··· / Report of Contributions

CuFe2O4/ reduced graphene oxid  $\cdots$ 

Contribution ID: 126

Type: Invited Talk

# CuFe2O4/ reduced graphene oxide nanocomposites: effect of synthesis conditions on structure, morphology, magnetic, electrical and electrochemical properties

Tuesday, November 5, 2024 1:40 PM (20 minutes)

Type of presence

**Presenter:** Prof. KOTSIUBYNSKYI, Volodymyr (Vasyl Stefanyk Precarpathian National University, Ivano-Frankivsk)

Session Classification: Workshop on Sustainable Materials and Technologies

Perovskite-based electrode mater ...

Contribution ID: 127

Type: Invited Talk

# Perovskite-based electrode materials for solid oxide fuel cells

*Tuesday, November 5, 2024 11:00 AM (20 minutes)* 

Type of presence

**Presenter:** Dr KOLKOVSKYI, Pavlo (Vasyl Stefanyk Precarpathian National University)

Session Classification: Workshop on Sustainable Materials and Technologies

Short Intro about the creation of a  $\cdots$ 

Contribution ID: 128

Type: Oral

### Short Intro about the creation of a maskless lithography lab in Kyiv in the framework of the NRFU project

Wednesday, November 6, 2024 8:15 AM (10 minutes)

Type of presence

**Presenter:** Prof. DZHAGAN, Volodymyr (Lashkaryov Institute of Semiconductor Physics (ISP), NAS of Ukraine)

Interference nanolithography bas ...

Contribution ID: 129

Type: Invited Talk

# Interference nanolithography based on chalcogenide photoresist

Wednesday, November 6, 2024 8:25 AM (20 minutes)

Type of presence

**Presenter:** Dr DAN'KO, Viktor (Lashkaryov Institute of Semiconductor Physics (ISP), NAS of Ukraine)

Laser Beam Lithography at Raith …

Contribution ID: 130

Type: Oral

# Laser Beam Lithography at Raith Laser Systems BV

Wednesday, November 6, 2024 10:00 AM (20 minutes)

Type of presence

Presenter: Dr KESKINBORA, Kahraman (Raith Laser Systems BV)

Type: Oral

# Spectral stability of CsPbX3 (Br, I) perovskite nanocrystal for single photon emission

Tuesday, November 5, 2024 11:40 AM (15 minutes)

In 2015, Park and colleagues generated the first room temperature perovskite based single-photon source using all-inorganic CsPbI3 quantum dots (QDs). Since then, quantum light emission from a variety of perovskite nanocrystals (PNCs) has been demonstrated at both ambient and cryogenic temperatures. Despite the remarkable features of PNCs, the use of PNCs is restricted by their photostability. The research focus has moved to their challenging integration into photonics platforms. In this study, we utilized cryogenic micro-PL and micro-TRPL spectroscopy to investigate the spectral stability, blinking, and spectral color purity of single colloidal cesium lead halide PNCs with different caping ligands. Compared to typical oleic amine/oleic acid (OLA/OA) ligands, PNCs capped with zwitterionic (ZW) ligands exhibited a significant reduction in blinking effect, along with strong linewidth narrowing and enhanced spectral stability. Additionally, a slightly longer decay time (by a factor of ~1.35) was observed for CsPbBr3 single NCs with ZW ligands, indicating a reduction in undesirable effects such as Auger recombination, making these NCs better suited for single-photon sources. However, for CsPbI3 PNCs, this strategy was ineffective, and traditional OLA/OA ligands remained the best option. For CsPbI3 NCs, we measured a second-order photon correlation function of g2(0) ~0.3, confirming their suitability for single-photon emission. Furthermore, spectral diffusion effect was significantly reduced in both single CsPbBr3 PNCs with ZW ligands and CsPbI3 PNCs with OLA/OA ligands, resulting in narrow micro-PL linewidths of ~125 µeV and ~140 µeV, respectively. Our findings pave the way for utilizing perovskites and single photon sources as key components in quantum technology-oriented applications.

### Type of presence

**Primary author:** Dr GORJI, Setatira (Institut de Ciència dels Materials (ICMUV), Universitat de València. Catedrático José Beltrán 2, 46980 Paterna, Valencia, Spain.)

**Presenter:** Dr GORJI, Setatira (Institut de Ciència dels Materials (ICMUV), Universitat de València. Catedrático José Beltrán 2, 46980 Paterna, Valencia, Spain.)

Session Classification: Workshop on Sustainable Materials and Technologies

Type: Oral

### Optical Emulation of Rabi coupling for Sensing Applications

Friday, November 8, 2024 9:20 AM (15 minutes)

Optical systems are at the forefront of modern technologies, from telecommunications to quantum computing, offering unparalleled speed and efficiency in data processing and transmission. To develop and optimize these systems, engineers and scientists rely on tools like optical emulators. These tools play a critical role in modeling, testing, and refining optical networks, devices, and phenomena before real-world implementation. Optical emulators are light-based systems that mimic the behavior of physical devices and networks, providing an efficient way to test and optimize performance in real-time scenarios. This presentation explores the phenomenon of Rabi-like splitting based on mode-mode coupling and self-referenced refractive index sensing using an open-access microcavity setup. Here, we investigate the coupling between cavity photon modes and optical Bragg modes arising from distributed Bragg reflectors (DBRs). By tuning the cavity length, cavity photon modes can be detuned to hybridize with Bragg modes, resulting in observable anticrossing at distinct Bragg mode positions, validating the strong coupling between the modes and producing tunable Rabi-like splitting energies. This coupling strength can be adjusted by depositing an active absorber layer on one of the cavity mirrors, with further control achieved by optimizing the thickness of the absorber material and fine-tuning the cavity length. The strong coupling and mode hybridization were experimentally observed and corroborated through numerical modeling using finite element methods (FEM). These hybrid modes provide a novel mechanism for designing selfreferenced refractive index sensors, capable of detecting various analytes with high sensitivity. The open-access nature of this cavity configuration allows for seamless integration in applications ranging from biological sensing to quantum measurements, positioning it as a versatile tool for future sensing technologies.

### Type of presence

**Primary author:** Dr PASHAEI ADL, Hamid (Institut de Ciència dels Materials (ICMUV), Universitat de València. Catedrático José Beltrán 2, 46980 Paterna, Valencia, Spain.)

**Presenter:** Dr PASHAEI ADL, Hamid (Institut de Ciència dels Materials (ICMUV), Universitat de València. Catedrático José Beltrán 2, 46980 Paterna, Valencia, Spain.)

Session Classification: Quantum Optics and Photonic Information Processing

Advanced Maskless Lithography …

Contribution ID: 133

Type: Oral

# Advanced Maskless Lithography Techniques for High-Precision Microstructure Fabrication

Wednesday, November 6, 2024 10:20 AM (15 minutes)

Type of presence

**Primary author:** Dr KALENYUK, Oleksii (G.V. Kurdyumov Institute for Metal Physics, N.A.S. of Ukraine, Kyiv Academic University)

**Presenter:** Dr KALENYUK, Oleksii (G.V. Kurdyumov Institute for Metal Physics, N.A.S. of Ukraine, Kyiv Academic University)

25TH SYMPOSI ··· / Report of Contributions

How to start business in optics

Contribution ID: 134

Type: Invited Talk

# How to start business in optics

Thursday, November 7, 2024 10:30 AM (20 minutes)

Primary author: Dr MELENEVSKY, Dmytro (Novazii LLC)

**Presenter:** Dr MELENEVSKY, Dmytro (Novazii LLC)

**Session Classification:** Professional Development in Optics: Navigating Opportunities and Entrepreneurship

Luminescent carbon dots: critical ···

Contribution ID: 135

Type: Invited Talk

# Luminescent carbon dots: critical review

*Tuesday, November 5, 2024 3:00 PM (20 minutes)* 

**Presenter:** Dr VASIN, Andrii (Lashkaryov Institute of Semiconductor Physics, Kyiv Ukraine) **Session Classification:** Workshop on Sustainable Materials and Technologies

Type: Oral

### Femtosecond Optical Kerr Effect for Biological Application

Friday, November 8, 2024 2:20 PM (15 minutes)

The Optical Kerr Effect (OKE) is a non-linear optical phenomenon in which an intense electric field induces a birefringence in the sample causing changes to the non-linear index (n2). The OKE is attributed to the distortion of the bound and free electrons and the disturbance of the molecular motions in a material.

Our work proposes the OKE as a potentially new method to differentiate differet types of tissues through key biomarkers from the temporal profile. The primary biomarker observed in our study comes from the double peak temporal Kerr structure signal, which we first observed in breast chicken tissue and human brain tissue. The second and most important biomarker is the doubling in the tissue's conductivity. For example, a cancerous breast tissue was shown to be about twice as conductive as healthy tissue depending on its grade. In general, our finding suggests conductivity from electrons and ions in plasma in a tissue can be used as a new major biomarker for the classification or detection of diseases. Our methods can be potentially used for differentiating other diseases such as neurological diseases.

### Type of presence

**Primary author:** Dr MAMANI, Sandra (Institute for Ultrafast Spectroscopy and Lasers, Departments of Physics and electrical Engineering, The City College of the City University of New York, 160 Convent Avenue, New York, NY 10031, USA)

**Presenter:** Dr MAMANI, Sandra (Institute for Ultrafast Spectroscopy and Lasers, Departments of Physics and electrical Engineering, The City College of the City University of New York, 160 Convent Avenue, New York, NY 10031, USA)

Session Classification: Biomedical Imaging and Nanotechnology

Femtosecond and Nanosecond La ...

Contribution ID: 137

Type: not specified

# Femtosecond and Nanosecond Laser Technology for Material Research (Фемто та наносекундна лазерна техніка для дослідження матеріалів )

Thursday, November 7, 2024 3:00 PM (1h 30m)

**Presenter:** Prof. DMYTRUK, Igor (Faculty of Physics, Taras Shevchenko National University of Kyiv, Ukraine)

Session Classification: School on Advanced Optical Materials

25TH SYMPOSI ··· / Report of Contributions

Extraction of Equivalent Paramet ...

Contribution ID: 138

Type: not specified

# Extraction of Equivalent Parameters of Barrier Structures from Current-Voltage Characteristics (Вилучення еквівалентних параметрів бар'єрних структур з вольт-амперних характеристик)

Wednesday, November 6, 2024 3:00 PM (1h 30m)

Primary author: Prof. OLIKH, Oleg (Taras Shevchenko National University of Kyiv)Presenter: Prof. OLIKH, Oleg (Taras Shevchenko National University of Kyiv)Session Classification: School on Advanced Optical Materials

25TH SYMPOSI ··· / Report of Contributions

Atomistic Modeling of Thermal T

Contribution ID: 139

Type: not specified

# Atomistic Modeling of Thermal Transport Processes in Nanomaterials (Атомістичне моделювання процесів теплового транспорту в наноматеріалах)

Wednesday, November 6, 2024 4:30 PM (1h 30m)

Presenter: Dr KURYLIUK, Vasyl (Taras Shevchenko National University of Kyiv, Kyiv, Ukraine)

Session Classification: School on Advanced Optical Materials

Metamaterials: Theory and Appli  $\,\cdots\,$ 

Contribution ID: 140

Type: not specified

# Metamaterials: Theory and Applications (Метаматеріали. Теорія та застосування.)

Friday, November 8, 2024 4:30 PM (1h 30m)

Primary author: Dr KOZACHENKO, Viktor (Taras Shevchenko National University of Kyiv)
Presenter: Dr KOZACHENKO, Viktor (Taras Shevchenko National University of Kyiv)
Session Classification: School on Advanced Optical Materials

25TH SYMPOSI ··· / Report of Contributions

Unique Properties of Laser Radia ...

Contribution ID: 141

Type: not specified

# Unique Properties of Laser Radiation and Its Applications in Science and Technology (Унікальні властивості лазерного випромінювання і застосування його в науці і техніці)

*Friday, November 8, 2024 6:00 PM (1h 30m)* 

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