# 26TH SYMPOSIUM ON PHOTONICS AND OPTICS SPO 2025

Wednesday 5 November 2025 - Friday 7 November 2025 Zoom and Faculty of Physics, Taras Shevchenko National University of Kyiv, Kyiv, Ukraine

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#### Biophotonics & Molecular Spectroscopy / 189

### Measuring all-protein concentration in DNA repair foci by FLIM

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On average one cell suffers up to tens of thousands of DNA lesions per day, induced by endogenous and environmental factors [1-3]. Induction of DNA damage leads to the recruitment of repair factors and formation of a DNA repair focus. It is reasonable to expect that the numerous repair factors that are recruited to a damaged site transiently create a distinct local microenvironment surrounding a DNA lesion. Despite the seemingly stable nature of repair foci (DSB repair foci may last for hours, and SSB for several minutes or longer), repair proteins recruited to DNA damage are dynamic, continuously exchanging with the surrounding nucleoplasm throughout the repair process. Thus, an intriguing question arises as to the actual total concentration of all proteins residing in a repair focus and the role of high molecular crowding in creating an environment conducive to effective repair. Using fluorescence lifetime imaging (FLIM), we demonstrated that repair foci that are formed in response to DNA breaks are much more densely packed with proteins than the surrounding nucleoplasm [4]. According to our data the local concentration of all proteins (i.e., the residing and recruited ones) in double- and single-strand DNA repair foci can be even 2.2 times higher than that in the surrounding nucleoplasm, which brings them close to the achievable maximum concentration. We hypothesize that a microenvironment characterized by such a high protein concentration may facilitate the formation of protein condensates, resulting in the stabilization of repair complexes.

- 1. Lindahl, T., Instability and decay of the primary structure of DNA. Nature 1993, 362 (6422), 709-15.
- 2. De Bont, R.; van Larebeke, N., Endogenous DNA damage in humans: a review of quantitative data. Mutagenesis 2004, 19 (3), 169-85.
- 3. Yousefzadeh, M.; Henpita, C.; Vyas, R.; Soto-Palma, C.; Robbins, P.; Niedernhofer, L., DNA damage-how and why we age? Elife 2021, 10.
- 4. Levchenko, S. M.; Dobrucki, J. W., High Molecular Crowding in Repair Foci Surrounding DNA Breaks, Measured by Fluorescence Lifetime Imaging Microscopy. Faseb Journal 2025, 39 (17).

#### Type of presence:

Presence online

**Biophotonics & Molecular Spectroscopy / 176** 

# **Spectral Investigations of Indole-Containing Organic Compounds for Biomedical Drugs**

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The indole-containing organic compounds represent a unique class of substances due to their broad biomedical activity such as antibacterial, antiviral, anti-inflammatory, and anticancer. Our ongoing study presents the design, synthesis, and spectral analysis of novel indole-containing compounds, specifically indolo[2,3-b]quinoxaline and indolo[2,1-b]quinazoline-6,12-dione derivatives, targeted for biomedical applications mentioned above.

The synthesized compounds underwent rigorous photophysical characterization. The absorption spectra were recorded on a Cary 60 (Agilent) UV-Vis spectrophotometer, the fluorescence and phosphorescence spectra were analyzed using a Cary Eclipse (Varian) fluorescent spectrophotometer, which was also used for low-temperature measurements. This extensive experimental dataset was correlated with theoretical calculations performed using Gaussian'16, which modeled the electronic structures and optical properties of the compounds. This combined approach allowed for a deep understanding of the reasons how the chemical structure influences the photophysical behavior, which is critical for designing effective DNA intercalators or photosensitizers [1, 2].

This research expands the class of functional organic compounds with defined photophysical characteristics, establishing a foundation for their development as potential pharmaceuticals, such as DNA intercalators for cancer therapy or novel antimicrobial agents.

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[1] Kudrya, V. Y.; Zhang, T.-Y.; Tan, M.-X.; Naumenko, A. P. Spectro-Luminescent characterization [2] SHARMA, B. K.; SHAIKH, A. M.; CHACKO, S.; KAMBLE, R. M. Synthesis, Spectral, Electrochemical as
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#### Type of presence:

Presence at Taras Shevchenko National University

Connecting Ukrainian Science to Europe's Research Infrastructures / 193

#### The talk title will be announced later

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Type of presence:

Connecting Ukrainian Science to Europe's Research Infrastructures / 183

### German–Ukrainian Scientific Cooperation: The Role of DESY and DZA

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In recent years, Germany has played a key role in supporting Ukrainian science, particularly in the fields of physics, astrophysics, and research infrastructure development. The Deutsches Elektronen-Synchrotron (DESY) plays a significant part in this process as Germany's leading national laboratory for accelerator physics, photon science, and astroparticle research.

Since the beginning of the full-scale war, DESY has been among the first European institutions to join targeted initiatives supporting Ukrainian researchers, including the Ukrainian EURIZON program, and has recently joined the newly established Research Infrastructures for the Future of Ukraine

<sup>&</sup>lt;sup>1</sup> German Center for Astrophysics and DESY

(RIFF) platform. Moreover, DESY organizes annual DESY–Ukraine Summer Schools and training programs for Ukrainian students and scientists.

In 2024–2025, this cooperation has expanded to include the Deutsches Zentrum für Astrophysik (DZA) —a newly established national center for science, technology, and innovation located in Görlitz. The DZA focuses on astronomy, digitalisation, and cross-border collaboration in Eastern Europe. Together, DESY and DZA contribute to the Recovery of Ukrainian Astronomy initiative, aligned with the Rome Declaration of Intent for Science, Research, and Innovation in Ukraine (2023). The goal is to restore scientific infrastructure, strengthen researcher mobility, and reintegrate Ukrainian science into the European Research Area (ERA).

From DZA's perspective, this cooperation extends beyond institutional partnerships and aims to connect Ukrainian researchers with Europe's next-generation scientific infrastructures —including the Einstein Telescope, a planned underground interferometric observatory that will use advanced laser and photonics technologies to detect gravitational waves with unprecedented sensitivity. Such projects exemplify the deep synergy between astrophysics and photonics and underline the importance of international collaboration in advancing fundamental science.

Looking ahead, DESY and DZA aim to further strengthen German–Ukrainian collaboration, ensuring Ukraine's participation in major international scientific projects and fostering the development of a sustainable, interconnected European research landscape.

#### Type of presence:

Presence online

Functional Oxides, Glasses & Thin-Film Processing / 150

### Structural, Microstructural, and Dielectric Properties of Ba(2–x)Sr(x)GdFeNb<sub>4</sub>O<sub>15</sub> Ceramics with Tetragonal Tungsten Bronze Structure

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Lead-free ferroelectric materials with a tetragonal tungsten bronze (TTB) structure have attracted increasing attention due to their multifunctional potential in microelectronics and energy applications. In this study, Ba(2–x)Sr(x)GdFeNb<sub>4</sub>O<sub>15</sub> (x = 0, 1, 2) ceramics were synthesized via the solid-state reaction route to investigate the influence of Sr substitution on structural and dielectric behaviors. X-ray diffraction combined with Rietveld refinement confirmed the formation of a single TTB phase with space group P4/mbm, showing a systematic decrease in lattice parameters with increasing Sr content, attributed to the smaller ionic radius of Sr<sup>2+</sup> compared to Ba<sup>2+</sup>. Raman and FTIR spectroscopies evidenced characteristic vibrational modes of the MO<sub>6</sub> octahedra, reflecting subtle structural distortions upon substitution. SEM analysis revealed dense microstructures with grain sizes varying from 2 to 14  $\mu$ m, depending on the Sr concentration. Dielectric measurements demonstrated a high dielectric constant, low losses, and a sharp permittivity peak near the Curie temperature ( $\approx$ 310–330 °C), typical of classical ferroelectric behavior. The Curie–Weiss analysis indicated a second-order phase transition with large Curie constants (C > 10<sup>4</sup>), confirming the displacive nature of the transition. These findings highlight the significant tunability of TTB-type Ba–Sr–Gd–Fe–Nb oxides for potential applications in capacitors, sensors, and multifunctional electronic devices.

#### Type of presence:

Presence online

#### Functional Oxides, Glasses & Thin-Film Processing / 166

### Structural and Optical Features of Molybdenum-Doped Phosphate Glasses

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The study focuses on the synthesis and characterization of phosphate and borate glass systems modified with transition metal oxides such as molybdenum and tungsten. The incorporation of these oxides was found to influence the short- and medium-range structure of the glass network, leading to changes in coordination states and connectivity of structural units. Subsequent doping with europium ions was carried out to investigate the sensitization effects and energy transfer processes in isotropic glassy media. The optical and luminescence properties were examined using UV–Vis and photoluminescence. The obtained results demonstrate the role of transition metal oxide modifiers in enhancing local field effects and facilitating nonradiative energy transfer to Eu<sup>3+</sup> centers, resulting in improved emission intensity and color purity. These findings contribute to understanding the structure–property relationships in oxide glasses and provide insight into the design of new luminescent materials for photonic and optoelectronic applications

#### Type of presence:

Presence at Taras Shevchenko National University

#### Functional Oxides, Glasses & Thin-Film Processing / 169

### Structural studies of As-S-Se glasses

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Structural studies of As-S-Se glasses

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The mid-IR photonics sector uses chalcogenide As-S-Se glasses extensively. These glasses are used in a variety of applications, including optical fibres for power delivery and supercontinuum generation, as well as sensing and spectroscopy. They can be used as inorganic photoresists, holography media, in fabrication of optical elements such as axicons and Fresnel zone plates.

In this work, three compositions of the As-S-Se system -  $As_{32.39}S_{62.70}Se_{4.91}$ ,  $As_{41.24}S_{27.11}Se_{31.65}$ , and  $As_{43.29}S_{26.15}Se_{30.56}$  - were investigated using X-ray diffraction. The measurements were performed with a Rigaku SmartLab diffractometer in parallel-beam geometry employing Cu K $\alpha$  radiation ( $\lambda$  = 1.5406 Å) within the 2 $\theta$  range of 2-120° and a step size of 0.05° at room temperature. The radial distribution functions (RDFs) were calculated using RAD GTK+, yielding first-neighbour distances  $r_1$  ranging from 2.29 to 2.40 Å, which fit well within the values typically reported for chalcogenide As-S/Se networks.

Complementary Raman spectroscopy measurements were carried out using a LabRAM HR spectrometer (HORIBA Scientific) in backscattering geometry at room temperature. The spectra were excited with a 514.7 nm laser (110  $\mu W)$  focused through a 50x objective, covering the 50-1500 cm $^{-1}$  spectral range with 1 cm $^{-1}$  resolution and an integration time of 120s. The obtained vibrational bands are

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consistent with those reported in the literature for As-S-Se glasses, confirming the presence of mixed  $AsS_{3/2}$  and  $AsS_{9/2}$  pyramidal units.

#### Type of presence:

Presence at Taras Shevchenko National University

Functional Oxides, Glasses & Thin-Film Processing / 184

# Tailoring the Optical and Structural Properties of Si-Doped HfO<sub>2</sub> Films by Hydrogen-Assisted Magnetron Sputtering and Post-Annealing treatment

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The optical and structural properties of Si-doped HfO2 thin films were systematically investigated as a function of deposition conditions and post-deposition annealing. The films were deposited by RF magnetron sputtering of a composite Si:HfO<sub>2</sub> target in pure Ar or Ar-H<sub>2</sub> plasma. Structural, optical, and luminescent characteristics were examined using spectroscopic ellipsometry, photoluminescence, Fourier transform infrared spectroscopy, and transmission electron microscopy. The Si content in the films was controlled either by varying the Si:HfO<sub>2</sub> target composition or by adjusting the hydrogen flow during sputtering. The former approach increased the refractive index up to 2.42 (at 1.95 eV), while hydrogen incorporation further enhanced it to about 2.7, compared with 1.98-2.00 for undoped HfO<sub>2</sub>. Annealing in nitrogen at 400-900 °C preserved the amorphous and chemically homogeneous structure, demonstrating high thermal stability and suitability for optical device integration. At higher annealing temperatures (up to 1100 °C), phase separation occurred, leading to the formation of distinct HfO2 and SiO2 phases. Alternating deposition in Ar and Ar-H<sub>2</sub> plasmas enabled the fabrication of multilayered Si-doped structures from a single composite target, allowing controlled variation of the sublayer composition. For films with elevated Si content, a narrow processing window was identified that favored the formation of highly Si-rich phases. These results revealed the promising properties of Si-doped HfO<sub>2</sub> materials for tunable optical applications.

#### Type of presence:

Presence online

Perovskites & Semiconductor Devices (PV/LED) / 195

### Self-assembled growth of high-quality InGaN 'lotus seed pod'structures with red emission

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Anisotropic epitaxial growth of free-standing InGaN nanostructures remains a key technological challenge in light-emitting device development. Here, we report precise, stepwise control of InGaN nanostructure growth on Si(111) substrates using molecular beam epitaxy (MBE). Light nitridation of the Si(111) surface created nucleation centers that promoted the well-oriented formation of hexagonal InGaN structures. Under nitrogen-rich conditions with a III/V flux ratio of 1.2, high indium incorporation up to 68% was achieved. This approach enabled the self-assembly of InGaN nanotowers with a distinctive 'lotus seed pod'morphology, reaching heights of up to 650 nm. Growth kinetics were monitored at each stage via reflection high-energy electron diffraction (RHEED), ensuring precise control over structure formation. Photoluminescence measurements at room temperature revealed a pronounced red emission peak at 705 nm, demonstrating the optical quality and potential applicability of these structures. The combination of controlled morphology, high indium incorporation, and efficient red emission indicates that self-assembled InGaN 'lotus seed pod'nanostructures are promising candidates for next-generation light-emitting devices.

#### Type of presence:

Presence online

Perovskites & Semiconductor Devices (PV/LED) / 146

### Structural and Optical Properties of Aziridinium Germanium Hybrid Perovskites

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Hybrid halide perovskites containing small organic cations continue to attract attention as semiconducting materials for optoelectronic applications, which make them promising candidates for nextgeneration photovoltaic and optoelectronic devices. Among them, aziridinium-based perovskites represent an emerging class of compounds with distinctive structural and optoelectronic properties, enabling the formation of stable three-dimensional perovskite frameworks.[1, 2] In the present work, a series of germanium-based hybrid perovskites with the general formula (AzrH)GeX3 (X = Cl, Br) were synthesized and comprehensively studied. Single-crystal X-ray diffraction analysis revealed that (AzrH)GeCl3 crystallizes in the *Pnma* space group and (AzrH)GeBr3 crystallizes in *R3m* space group at room temperature and are characterized by a non-centrosymmetric crystal structure -a distinctive feature that may open opportunities for nonlinear optical applications. Differential scanning calorimetry (DSC) and variable-temperature X-ray diffraction measurements indicate the presence of temperature-induced phase transitions. Optical diffuse reflectance spectroscopy was used to determine the band gap values by the Kubel'ka-Munk method, which were found to be 3.18 eV for (AzrH)GeBr3 and 3.87 eV for (AzrH)GeCl3. These results allow us to classify the materials as wide-band-gap semiconductors. The obtained data extend the family of aziridinium-based perovskites and demonstrate that germanium substitution leads to significant changes in the structure and electronic characteristics compared to their lead and tin analogues.

- 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.

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#### Type of presence:

Presence online

Perovskites & Semiconductor Devices (PV/LED) / 157

# Aziridinium Cation as a Universal Building Block for HOIPs of Variable Dimensionality

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Hybrid organic-inorganic perovskites remain at the forefront of materials research due to their tunable optoelectronic properties and structural diversity. In this work, we present a family of aziridinium-based hybrid perovskite-like materials of general formula (AzrH)<sub>3</sub>M<sub>2</sub>X<sub>9</sub> (M = Sb, Bi; X = Cl, Br, I), where the aziridinium cation (AzrH)<sup>+</sup> acts as a versatile structure-directing template enabling the formation of perovskite of all dimensionalities—0D, 1D, 2D, and even 3D.1 Single-crystal X-ray diffraction revealed discrete bi-octahedral 0D units in iodides, 1D polymeric chains in antimony chloride, and layered 2D structures in bromides and bismuth chloride. Furthermore, heterovalent Bi<sup>3+</sup> doping in aziridinium lead halides enabled the stabilization of mixed-metal 3D perovskites with the band gap of 1.49 eV, which is the lowest value observed for this raw of materials. Across the (AzrH)<sub>3</sub>M<sub>2</sub>X<sub>9</sub> series, the optical absorption features strong excitonic transitions (330–499 nm) with binding energies ranging from 0.06 to 0.61 eV, and band gaps varying from 2.61 to 4.09 eV depending on the halogen and metal composition. Density functional theory calculations support these findings, showing that valence and conduction band edges are primarily derived from halide p- and metal s-orbitals, respectively. The established correlations among dimensionality, composition, and optical behavior provide valuable insights into the design of hybrid perovskites with controllable electronic structures.

(1) Kucheriv, O. I.; Semenikhin, O. A.; Bibik, Y. S.; Bardyk, I.; Shova, S.; Gural'skiy, I. A. Aziridinium Cation as a Versatile Template for Hybrid Organic–Inorganic Perovskites of All Dimensionalities. Inorg. Chem. Front. 2025. https://doi.org/10.1039/d5qi01090j.

#### Type of presence:

Presence online

Perovskites & Semiconductor Devices (PV/LED) / 161

### 2D Hybrid Perovskite with Narrow-Band Violet-Blue Emission

Authors: Valerii Sirenko<sup>1</sup>; Olesia Kucheriv<sup>1</sup>; Dina Naumova<sup>1</sup>; Sergiu Shova<sup>2</sup>; Il'ya Gural'skiy<sup>1</sup>

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Hybrid organic-inorganic perovskites constitute a rapidly-growing family of solid-state semiconducting materials with remarkable potential in optoelectronic and photovoltaic applications. Their

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highly-tunable chemical composition enables emission across a broad spectral range; however, efficient violet-blue emitting perovskites remain relatively scarce. In this work, we present the synthesis, structural characterization, and optical properties of a new two-dimensional (2D) hybrid perovskite, (ethylammonium)2CdBr4. The crystal structure of this compound comprises infinite inorganic 2D layers formed by corner-sharing [CdBr6]4– octahedra, separated by ethylammonium cations. Optical absorption measurements indicate a wide band gap of 4.25 eV. Photoluminescence studies reveal a sharp emission peak centered at 388 nm with a full-width at half maximum (FWHM) of 32 nm, corresponding to chromaticity coordinates that closely approach the NTSC blue standard. Density functional theory (DFT) calculations of the electronic band structure and density of states (DOS) confirm that the states near the Fermi level are primarily derived from cadmium and bromine orbitals. The combined experimental and theoretical results demonstrate that (ethylammonium)2CdBr4 represents a promising candidate for violet-blue light emission, offering a simple, cost-effective route toward next-generation perovskite-based luminophores utilizing readily available organic cations. This study contributes to the ongoing exploration of low-dimensional perovskites as tunable emitters for advanced optoelectronic technologies.

#### Type of presence:

Presence online

Perovskites & Semiconductor Devices (PV/LED) / 145

# Backside surface engineering for improved performance of CIGS and CZTS solar cells: application of titanium dioxide (TiO) and graphene oxide (rGO) layer

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This work was conducted at the Ben M'Sik Faculty of Sciences, Engineering and Materials Laboratory (LIMAT) (Nanomaterials and Thin Films Team). This study is part of research efforts aimed at addressing global energy challenges. These challenges are caused in particular by rapid population growth, increased urbanization, and exponential energy demand. Faced with the progressive depletion of fossil resources and their environmental impacts, renewable energies, and solar energy in particular, are positioning themselves as an essential solution for a sustainable energy supply.

The main objective of this thesis is to optimize the performance of CIGS (Copper-Indium-Gallium-Selenium) and CZTS (Copper-Zinc-Tin-Sulfur) solar cells by making modifications to their internal layers. These modifications were analyzed using numerical simulations performed with SCAPS (Solar Cell Capacitance Simulator) software. Particular attention was paid to the integration of new materials for functional layers, including reduced graphene oxide (rGO) as the back surface field (BSF) layer and titanium dioxide (TiO2) as the buffer layer, to improve performance, reduce costs, and adopt a more environmentally friendly approach.

The experimental approach followed several steps: GO synthesis using a modified Hummers method, its chemical reduction to rGO using aluminum foil and hydrochloric acid, then the deposition of molybdenum thin films on soda-lime glass substrates by RF magnetron sputtering, and finally, the deposition of rGO in thin layers using techniques such as doctor blade and spin coating.

In parallel, CZTS-based structures were developed, integrating an rGO BSF layer and a TiO2 buffer layer. These devices were characterized using various techniques, such as X-ray diffraction (XRD), scanning electron microscopy (SEM), and Fourier transform infrared spectroscopy (FTIR), to assess their structural, morphological, and chemical properties.

This work is part of a dynamic research and innovation effort aimed at designing high-efficiency, stable, environmentally friendly photovoltaic cells compatible with industrial production. It was conducted in collaboration with the Department of Civil, Environmental, and Mechanical Engineering at the University of Trento (Italy).

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#### Type of presence:

Presence online

Perovskites & Semiconductor Devices (PV/LED) / 149

# Mn-Doped BaSnO<sub>3</sub> Perovskites for Next-Generation Optoelectronics: A First-Principles Investigation

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Perovskite oxides with the general formula ABO<sub>3</sub> offer highly tunable physical properties through substitution at the A and B lattice sites. In this work, manganese (Mn) was introduced into BaSnO<sub>3</sub> to evaluate its impact on structural, electronic, and optical properties. First-principles calculations were performed using density functional theory (DFT) within the pseudopotential plane-wave (PP-PW) framework implemented in Quantum Espresso for BaSn<sub>1-x</sub>Mn<sub>x</sub>O<sub>3</sub> (x = 0, 12.5, 25, and 37.5%). The lattice parameter decreases linearly with Mn incorporation, from 4.10 Å in pristine BaSnO<sub>3</sub> to 4.03 Å at x = 37.5%. The undoped compound exhibits a direct bandgap of 2.76 eV at the  $\Gamma$  point, which narrows significantly to 0.82 eV at 37.5% Mn doping due to enhanced Mn–O hybridization and altered orbital contributions within the valence band. Optical calculations reveal a progressive increase in the imaginary dielectric function  $\epsilon_2(\omega)$ , with static values rising from 0.07 (x = 0) to 3.21 (x = 37.5). This trend leads to marked enhancement of absorption coefficients, from 2.68 × 10<sup>5</sup> to 6.23 × 10<sup>5</sup> cm<sup>-1</sup> in the UV region and from 1.47 × 10<sup>5</sup> to 3.8 × 10<sup>5</sup> cm<sup>-1</sup> in the visible range, accompanied by a decrease in optical transmittance from ~80% to <76%. Overall, Mn doping enables precise tuning of the structural and optoelectronic response of BaSnO<sub>3</sub>, underscoring its promise for advanced optoelectronic applications.

#### Type of presence:

Presence online

Photonics, Lasers & Sensing / 154

### Performance Evaluation of the 'Cat-Eye' Effect Induced by a Laser System for Locating Optical Systems

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The increasing availability, ease of deployment, and simple masking of optical surveillance systems persistently raise the challenge of detecting such systems. This study explores the potential of active detection based on the retroreflection (cat-eye) effect, even under challenging illumination conditions such as bright daylight.

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The proposed method relies on active laser retroreflection, which produces a back-reflected signal from the target device's optical elements, thus enhancing detection efficiency. The analysis considers common surveillance optics, including smartphone cameras with apertures up to 2 mm and photographic lenses up to 20 mm in diameter. We assess the system's operational performance by calculating the maximum functional ranges based on the emitter's power.

The viability of this approach is confirmed by field experiments conducted over real atmospheric paths (up to 200 m), with results showing strong agreement with predictive computational models. The findings confirm that active retroreflection-based detection is a robust and practical tool for identifying concealed surveillance systems, even under the most challenging daylight conditions.

#### Type of presence:

Presence online

Photonics, Lasers & Sensing / 168

# Portable sensor platform based on plasmon-enhanced fluorescence for explosives detection

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The global challenge of rising terrorism has been further complicated by the war in Ukraine, which has led to extensive contamination of soil and water resources with explosives and their byproducts. This situation underscores the urgent need to develop a sensitive, rapid, low-cost, portable, and easily mass-produced sensor for explosive detection.

A promising approach for detecting various molecules is plasmon-enhanced fluorescence [1], which also shows potential for the detection of explosive molecules through the use of specific fluorophores [2]. In this work, new sensor fluorescent nanomaterials and a prototype of a portable sensor device for detecting molecules of a number of chemical analogs of explosive aromatic nitro compounds were developed.

Sensitive sensor elements based on the nanocomposites of fluorescent materials sensitive to explosives (pyrene, fluorene derivative F8BT, poly(phenylenevinylene) derivatives MEH-PPV and p-PMEH-PPV) with plasmonic nanostructures of noble metals in colloidal form and on substrates embedded into different polymer matrices, including acrylamide-based molecularly imprinted polymers, were prepared in the form of solid-state chips and paper-based carriers and characterized by microscopic and spectroscopic techniques to optimize their plasmon-enhanced fluorescence response. It was also found that pyrene and MEH-PPV fluorophores exhibit the highest fluorescence quenching against chemical analogs of explosive aromatic nitro compounds such as 4-nitrophenol and 4-nitrotoluene. The sensing properties of the prepared nanocomposites were investigated by analyzing fluorescence quenching response to different aromatic nitro compounds both in the gas and liquid phase to find their limits of detection, which reach 10-16 M for Ag nanoparticles/pyrene/polyvinylpyrrolidone thin films.

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

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#### Type of presence:

Presence online

Photonics, Lasers & Sensing / 170

### Quantitative Surface Texture Metrology via Single-Image Statistical Analysis of Laser Speckle

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Laser speckle, a phenomenon resulting from the scattering of coherent light from a rough surface, is rich with information encoding the surface's micro-topography. This work presents a novel optical methodology that decodes this information for quantitative, non-contact surface texture analysis from a single, static speckle. Our approach bypasses the temporal and mechanical constraints of traditional scanning profilometry by establishing a direct, quantitative correlation between the statistical properties of the speckle intensity field and surface texture parameters. The technique was experimentally confirmed using a set of industrially significant composite metal-ceramic samples. An optical configuration, comprising a He-Ne laser and a CMOS sensor, was used to capture far-field speckle patterns. Through rigorous cross-validation analysis, we demonstrate a strong correlation between speckle statistics and functional surface descriptors. Specifically, our model shows strong predictive power for Fractal Dimension and Gray-Level Co-occurrence Matrix (GLCM) Contrast, and accurately predicts surface Kurtosis. The sub-second acquisition-to-analysis pipeline underscores the technique's potential for high-throughput applications. This research validates a powerful, single-image optical approach, paving the way for compact, mechanically robust optical instruments for real-time, in-situ surface metrology.

#### Type of presence:

Presence at Taras Shevchenko National University

Photonics, Lasers & Sensing / 171

### Energy state of the electronic subsystem of porous carbon material caused by laser irradiation

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The influence of laser irradiation on the electrochemical properties of porous carbon material (PCM) doped with Er and Cr, as an electrode material of supercapacitors, was established from the analysis of impedance spectroscopy data. It has been experimentally shown that the specific capacitance of

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supercapacitors with electrodes of PCM doped with Er and Cr, increases by 40% and 60%, respectively. An increase in the Coulomb efficiency of supercapacitors formed on the basis of irradiated and doped with Er and Cr PCM has been established.

The PCM samples doped with Cr / Er were irradiated with a Nd:YAG laser. The pulse duration was  $\tau$  = 15 ns, the energy in the pulse was 0.01-0.015 J/cm2, the irradiation duration was T = 1.5-3 min, and the pulse repetition rate was f = 40-60 Hz. Thus, the choice of Er and Cr was due to the fact that they have a high density of electronic states near the Fermi level.

It is found that laser irradiation of Er and Cr-doped PCM increases the specific capacitance of supercapacitors formed on its basis by 40% and 60%, respectively. The internal resistance of Cr-doped PCM after laser irradiation grows by more than four times while remains practically unchanged for the Er-doped PCM. Also the Coulomb efficiency of Er/Cr-doped PCM supercapacitors practically does not change during first 105 charge/discharge cycles.

#### Type of presence:

Presence online

Photonics, Lasers & Sensing / 178

### Application of laser Doppler vibrometry for detection of objects buried in the soil

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Laser Doppler Vibrometry (LDV) is a modern technology for measuring mechanical vibrations of different amplitudes with high precision and without physical contact. It finds wide applications in industry, engineering, scientific research, biology, and medicine. The remote nature of LDV operation allows measurement of vibrations in hard-to-reach or hazardous locations. Specifically, it can be used for detection of explosive objects buried in the soil.

The work is aimed at development of laser-acoustic method for detection of buried mines in the context of humanitarian demining in Ukraine. In this method, the LDV registers vibrations of the soil surface (seismic waves) excited by external influences, in particular, sound waves generated by a loudspeaker. An explosive object buried at a depth of several centimeters is detected by a higher speed (higher amplitude) of soil vibrations above it compared to neighboring soil.

In this work, the design and operating principle of developed laser Doppler vibrometer, and setup of the laboratory stand of laser-acoustic complex for measurement of soil vibrations are examined. The acoustic response spectra of the soils of different types with buried plastic simulant of soviet anti-personnel mine ΠΜΗ-2 have been analyzed in a frequency range of 50-1000 Hz. It is shown that the acoustic characteristics of a soil-mine system depend on the presence of a buried object, construction of its upper casing, distance from it, as well as on the type of soil and its humidity. This fact should be considered when trying to recognize the mine by the oscillation frequency.

#### Type of presence:

Presence online

Plenary Session: USyNC and Synhrotron Research / 194

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### Introduction to Synchrotron Radiation and X-ray Free-Electron Lasers in Condensed Matter Research

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Type of presence:

Plenary Session: USyNC and Synhrotron Research / 185

### Synchrotron Light as a Tool to Unravel Luminescent Processes in Next-Generation Materials

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The application of synchrotron radiation light sources has revolutionized materials research by offering unique capabilities for studying the structure, electronic properties and energy relaxation dynamics of materials at unprecedented levels of detail. In particular, use of pulsed synchrotron radiation is the most efficient way to provide necessary time and energy resolution of the excitation in the VUV photon energy range. Luminescence arising from such excitation allows to study impurity/defect states, excitation energy transfer, elucidation of energy relaxation pathways and recombination mechanisms of electronic excitations, to study surface structure that is all together extremely important for study of the electronic structure and properties of materials with a wide bandgap.

#### Type of presence:

Presence online

Plenary Session: USyNC and Synhrotron Research / 191

# Ukrainian Synchrotron & Neutron Community and the Photonics of Quantum Materials

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Type of presence:

Presence at Taras Shevchenko National University

Poster Session / 144

### POLARITONS EXCITATED IN ZnO CERAMICS

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The report presents the results of studies on surface phonon and plasmon-phonon polaritons in undoped and manganese-doped ZnO ceramics for  $E \boxtimes c$  the orientation.

The authors obtained mathematical expressions for calculating the reflectance coefficient in the Attenuated Total Reflectance (ATR) spectra for undoped and manganese-doped ZnO ceramics in the frequency range of surface polariton (SP) excitation. Programs were developed to model and perform a dispersion analysis of the ATR spectra of the ZnO ceramics. Based on a quantitative analysis of the experimental and calculated spectra, the conditions under which experimental study of SP is possible were determined.

For the dispersion analysis of ATR spectra, a single-oscillator mathematical model was used, which additively accounts for the contribution of the phonon and plasmon subsystems to the dielectric permittivity of the ZnO ceramics. The calculations were performed for undoped and Mn-doped ZnO ceramics with different free carrier concentrations. In the frequency range between the transverse and longitudinal optical phonons of the ZnO ceramics, the theoretical and experimental dispersion dependencies and damping coefficients were investigated.

It is shown that the SP spectra for undoped and (manganese) doped ZnO ceramics are well modeled using mutually consistent parameters obtained by the authors for zinc oxide single crystals with orientation  $E \boxtimes c$ . This demonstrates the possibility of determining the optical and electrophysical parameters of ZnO ceramics (refractive index and absorption coefficient, plasma frequency and damping coefficient, etc.).

#### Type of presence:

Presence at Taras Shevchenko National University

#### Poster Session / 152

# Spectroscopic study of bovine serum albumin complexation with ibuprofen and silver nanoparticles

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Fluorescence quenching experiments were performed for aqueous BSA solutions at fixed protein concentration ( $2\,\mu\text{M}$ ) and varying ibuprofen concentrations in the range of  $0{\text -}1.5\,\mu\text{M}$  at three different temperatures (293, 303, and 313 K). Similar experiments were performed for aqueous solutions of BSA and ibuprofen with addition of Ar nanoparticles at fixed concentrations of ibuprofen and BSA and varying concentrations of nanoparticles.

Quenching behavior followed the Stern–Volmer relationship and revealed static quenching with binding constants increasing with temperature, suggesting a hydrophobic interaction mechanism. The calculated binding constants ranged from 4.3 to 5.0 with a binding stoichiometry close to 1:1. Thermodynamic analysis using the van't Hoff equation revealed positive values of  $\Delta H$  and  $\Delta S$ , confirming the spontaneous and entropy-driven binding.

Molecular docking simulations using AutoDock 4.2.6 identified three main binding clusters with 20 binding modes in total. The most energetically favorable modes are formed by all types of interactions (van der Waals, hydrogen-bonding, hydrophobic and electrostatic), but the most numerous are

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contacts with hydrophobic amino acid residues of BSA. The proximity of some binding modes to tryptophan residues supports the observed fluorescence quenching.

Acknowledgment

This work was supported by the National Research Foundation of Ukraine within the project "Nanostructural Modification of Application Drugs for Military Medical Technologies" (Grant No. 2023.04/0140).

#### Type of presence:

Presence online

Poster Session / 172

# Spectral properties of the new boron-containing dyes in composite thin films fabricated using thermal vacuum deposition method

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The development of organic light-emitting diodes (OLEDs) towards higher efficiency and lifetime depends on creating new efficient organic molecules which can be evaporated using thermal vacuum deposition method.

Here we present the studies of the electronic structure of new luminescent difluoroborate complexes of benz[c,d]indole derivatives. The one-component and composite Alq3-dyes thin films were fabricated using thermal vacuum deposition method.

The full interpretation of the absorption and fluorescence spectra of dyes solutions, one component and composite thin films has been done using the results of quantum-chemical calculations. The equilibrium molecular geometry and electronic structure of the lowest electron transitions of the dye molecules were performed on the software package Gaussians16 (DFT/B3LYP).

High fluorescence quantum yields of dyes in solutions and thin composite films can be explained by the calculated high dipole moments of first electron transitions and rigid molecule's structures. Efficient electron excitation energy transfer from the Alq3 matrix to dye molecules occurs at a dye concentration of about 1%. At the same time, these dyes have a low quantum yield in single-component thin films because of the formation of H-aggregates.

Due to high fluorescence quantum yields and good photostability the investigated compounds are promising candidates as emitters both in light-emitting layers of OLEDs and in sensor applications.

#### Acknowledgment

This work has received funding from the Ministry of Education and Sciences of Ukraine and Research Council of Lithuania, project "Exploitation of the solid-state enhanced long-lived emission of organic emitters for the detection of nitroaromatic explosive compounds"; agreements No S-LU-24-6, No M58-2024.

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#### Type of presence:

Presence at Taras Shevchenko National University

Poster Session / 158

# Analysis of dose-dependent luminescence of uncapped InGaAs quantum dots under 60Co γ-rays treatment

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We studied the influence of  $\gamma$ -irradiation on light-emitting characteristics (including intensity, peak position and half-width of photoluminescence bands) of the arrays of capped  $In_xGa_{1-x}As/GaAs$  QDs (x = 0.4) grown on GaAs (100) substrates. To reveal the radiation resistance of QDs we analyzed the dose-dependent variation of photoluminescence spectra after the treatment with  $\gamma$ -rays of  $^{60}$ Co source (doses varied in the range  $1 \div 10^3$  kGy range). Photoluminescence was excited using solid state laser with  $h\nu$  = 2.33 eV. Temperature dependences of photoluminescence spectra were registered in the temperature range 5 - 200 K.

It is shown that light emitting properties of the samples under study do not decline in the dose range up to  $10^3$  kGy, on the contrary, they even become better: the intensity of the photoluminescence slightly increases (about 60%) and FWHM remains almost constant. The observed effect can be interpreted in terms of the low dose effect - the model accounting for the improvement of crystalline structure under the irradiation with low doses of gamma rays. In this model the explanation of properties improvement is based on the interplay between pre-existing defects and radiation-induced defects that leads to the curing of non-radiative pathways for photoexcited carriers. Results on the temperature dependencies of the photoluminescence spectra support this interpretation: the activation energies of PL lines also remain unchanged under gamma-treatment. Thus, one can conclude that gamma treatment in the low dose range does not change the nature of light-emitting species while the sub-system of non-radiative defects undergoes quite noticeable changes.

Type of presence:

Poster Session / 160

### Methodology for microhardness profiling of composite materials

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Polytetrafluoroethylene (PTFE) is a synthetic thermoplastic polymer that significantly outperforms other polymer materials in terms of its anti-friction properties. Despite its advantages, polytetrafluoroethylene also has a number of disadvantages, such as a high thermal expansion coefficient and low mechanical strength. One promising way to overcome these disadvantages is to introduce various fillers into PTFE that comprehensively improve the properties of the polymer. The optimal set of properties is determined by the choice of filler based on its dispersion, surface topology, fillerto-polymer ratio, the technology used to mix the filler with the polymer, and the technology used to process the resulting composition into a product. Microhardness measurements have long been used as a method for microprobing the mechanical response of various materials and their compounds. Performing a series of microhardness measurements along a given line or on a given area on the surface of a sample allows for the development of a method for mapping or profiling of mechanical properties. Therefore, the aim of this work was to use a non-destructive instrumental indentation method to develop a microhardness profiling method for determining the effect of filler on the mechanical characteristics of a composite material. Nickel and silicon carbide particles were used as fillers for PTFE compositions in this work. The fillers were introduced into the fluoroplastic both separately and in various combinations, depending on the purpose of the compositions. The microhardness of the obtained materials was measured using the kinetic hardness method with a Micron-Gamma device, which allows simultaneous recording of the indenter penetration depth and load. The studies were conducted at loads ranging from 30 to 200 g according to the indenter loadingunloading scheme (without a pause between cycles). The change in microhardness was determined at different and constant loads on the indenter, depending on the indentation location. Graphs of the dependence of microhardness and Young's modulus on the load on the indenter were obtained. The study of the mechanical characteristics of composite materials, such as microhardness and Young's modulus, makes it possible to formulate a scientifically sound approach to predicting and targeting the properties of such composites.

#### Type of presence:

Presence at Taras Shevchenko National University

Poster Session / 177

### Modeling the Effect of Grain Reorientation on Crack Propagation in SiC

**Author:** Vadym Shvernyk None **Co-author:** Vasyl Kuryliuk 1

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The study of crack propagation in ceramics is critically important due to their widespread use in high-temperature and structural applications, where mechanical failure can lead to severe consequences. Silicon carbide (SiC) is particularly noteworthy because of its exceptional hardness and thermal stability; however, its brittleness necessitates a thorough understanding of fracture mechanisms. Molecular dynamics simulations have become a valuable tool for investigating crack dynamics at the atomic scale, offering insights that are difficult to achieve through experimental methods alone.

In this work, crack propagation was modeled in a SiC bicrystal, where one grain was rotated relative to the other by a specified angle to induce grain reorientation. Stress-strain curves were computed for bicrystal structures with varying reorientation angles, and the resulting crack paths were analyzed. The simulations demonstrate how grain misorientation influences both the mechanical response and the trajectory of crack propagation, providing crucial information for developing more fracture-resistant SiC-based materials.

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#### Type of presence:

Presence at Taras Shevchenko National University

Poster Session / 179

### Increasing the red emission of Mn4+ in magnesium aluminate by alloying with TiO2

Author: Lyudmyla Borkovska1

**Co-authors:** Kostyantyn Kozoriz  $^2$ ; Olexandr Gudymenko  $^2$ ; Igor Vorona  $^2$ ; Larysa Khomenkova  $^3$ ; Yevheniia Smortsova  $^4$ ; Alexander Welle  $^5$ ; Tetyana Kryshtab  $^6$ 

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Mn4+ activated oxides are highly stable, low cost and environmental safety materials that can be used as red phosphors in luminescence thermometry and phosphor-converted white light-emitting diodes. In MgAl2O4 spinel, the Mn4+ photoluminescence (PL) band with a peak at 651 nm is within human eye's sensitivity spectral range, but its luminous efficacy needs to be increased. In this work, the effect of alloying with TiO2 on optical and structural properties of Mn4+ activated MgAl2O4 ceramics produced by solid state reaction was studied. In the alloyed phosphors, the number of Al and Ti atoms was the same.

X-ray diffraction study of MgAl2O4:Mn ceramics revealed that concentration of spinel phase increased with annealing temperature up to 96% at 1400°C. In TiO2-alloyed ceramics, two crystalline phases of solid solutions were identified: spinel and qandilite, the concentration of former decreased and of latter increased with annealing temperature. In the PL spectra recorded under synchrotron radiation excitation, the PL bands caused by  $2E \rightarrow 4A2$  transition of Mn4+ in the Al2O3, MgAl2O4 and qandilite solid solution were identified. The CIE coordinates of MgAl2O4 and TiO2-alloyed ceramics were (0,6932, 0,2902) and (0,6953, 0,2894), respectively. The MgAl2O4:Mn ceramics also showed intense green PL caused by  $4T1 \rightarrow 6A1$  transitions of Mn2+. The presence of Mn2+ in MgAl2O4 host was confirmed by electron paramagnetic resonance study. The TiO2-alloyed ceramics demonstrated several times larger intensity of Mn4+ PL and no Mn2+ PL. It is concluded that alloying of MgAl2O4:Mn4+ with TiO2 is a promising approach for increasing the luminous efficacy of red phosphor.

#### Type of presence:

Presence online

Poster Session / 162

# Phase composition of coatings formed by the gas-detonation spraying of hydroxyapatite powder

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Recently, biocompatible coatings for medical implants have become widely used. To improve their functionality and safety, it is necessary to understand the mechanisms of coating formation. In this study we present an analysis of the phase composition of biocompatible coatings produced from hydroxyapatite (HA) powder using the gas-detonation spraying technique. The coatings were deposited onto various substrates, including metals (copper, medical, and technical titanium), quartz plates, and polymers (polyetheretherketone, fluoroplastic). Raman spectroscopy was employed for structural characterization. It was found that all studied coatings contain crystalline HA and additional (secondary) phases. It was shown that secondary phase depends on the substrate material, namely, for metal substrates it is amorphous HA, for polymer substrates it is tricalcium phosphate. The study of coatings with different thicknesses showed the formation of a transition layer between coating and substrate, which differs in phase composition from the main coating. In the case of polymer substrates, it is characterized by an increased tricalcium phosphate content, while for metal substrates the intermediate layer is determined by a reduced content of amorphous HA. In addition, it was observed that an increase in the distance between the gun and the metal substrate leads to a decrease in the content of amorphous HA in the coating. The obtained experimental data allow us to suppose a formation mechanism of the sprayed coatings based on the macro-characteristics of substrate material, namely, hardness and thermal conductivity.

#### Type of presence:

Presence at Taras Shevchenko National University

Poster Session / 173

### Peculiarities of microfibrillated and bacterial cellulose luminescence properties

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Cellulose is the most abundant natural polymer, with great potential to replace plastics in various human activities, including packaging, textiles, and electronics. The eco-friendliness, biodegradability, and low production costs are among the main advantages of the cellulose-based materials compared to common petroleum-based polymers. Recent studies indicated that cellulose and its derivatives can also be used as functional materials in modern high-tech electronics and optoelectronics, e.g., wearable flexible sensors, solar cells, energy storage systems, and organic light-emitting diodes. We report here the results of two types of cellulose materials'luminescence studies. The first type is Cotton Linter cellulose (commercial, purchased from Sigma Aldrich), which consists of microfibrils, and the second one is nanocellulose (produced by us), which was obtained through a bacterial process. It was found that both celluloses exhibit intense photoluminescence (PL) under PL excitation in the ultraviolet (UV) and visible spectral ranges (265-490 nm). In case of PL excitation at 265 nm, the PL spectra consist of several overlapping components with maxima near 331, 367, 407, 432, 494, and 577 nm, respectively. Although all these bands can be found in both of the studied celluloses, their relative intensities are different. This difference in the PL properties has been attributed to the distinct content of Ia and Ib cellulose phases in the studied samples. The PL kinetics studies have shown that each of the PL band consist of slow (milliseconds) and fast (microseconds) components, with increased contribution of the slow component for the long-wavelength emission.

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#### Type of presence:

Presence online

Poster Session / 174

# Luminescent properties of Eu ions doped (1-x)(27P<sub>2</sub>O<sub>5</sub>-36MoO<sub>3</sub>-5Bi<sub>2</sub>O<sub>3</sub>-32K<sub>2</sub>O)-xKBi(MoO<sub>4</sub>)<sub>2</sub> glasses and glass-ceramics

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Various oxide glasses and glass-ceramics have attracted significant attention as optical materials for applications in optoelectronics, such as displays, light-emitting diodes, temperature sensors, as well as active laser media. Some of glasses exhibit own photoluminescence (PL), but that emission is broadband, low intensity. Thus, it is therefore unsuitable for practical use. Doping with luminescent ions of transition or rare-earth metals enables significant improvement in the PL properties of glasses and glass-ceramics. Among the luminescent ions, the Eu³+ ones are known for their high PL intensity and narrow lines in the orange and red spectral regions (570 –730 nm). These ions are perfect luminescent probes for the crystal/atomic structure of materials, as  $^5D_0 \rightarrow ^7F_2$  electronic transitions are highly dependent (hypersensitive) on the symmetry of the local environment of the ion.

We report here our recent findings on the optical properties of  $27P_2O_5$ -36MoO<sub>3</sub>-5Bi<sub>2</sub>O<sub>3</sub>-32K<sub>2</sub>O glasses, both pure and Eu³+-doped, as well as glass-ceramics where the aforementioned glass is a host and powder of KBi(MoO<sub>4</sub>)<sub>2</sub>:yEu micro/nanocrystals is a filler. The undoped glasses reveal relatively weak PL in the ultraviolet and visible spectral regions. The spectra of the PL were ascribed to the emission centers formed by bismuth ions and MoO<sub>4</sub> tetrahedra. The clear difference in Eu³+- related emission spectra was observed for glasses, KBi(MoO<sub>4</sub>)<sub>2</sub>:yEu and glass-ceramics. This result can be explained by the formation of an interphase layer in the glass-ceramics with a specific chemical composition and characteristic optical properties.

#### Type of presence:

Presence online

Poster Session / 159

# Ag/Au nanoparticles of different shape for SERS detection of nitro group compounds

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SERS, owning to it advantageous combination of ultra-sensitivity, high speed, low costs, multiplexing capability, and portability, may be a key method for explosives detection. The core of the SERS-based detection is the SERS-substrate –a specially designed nanostructured surface of noble metal, with a large number of "hot spots"–places nigh local concentration of electric field, generated by laser excitation.

In this work, we synthesized Au and Ag nanoparticles of different shapes (spherical, cubic, elliptical

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etc) and sizes (10-60nm). Sizes and shapes of investigated NPs were confirmed by DLS and SEM measurements. From optical absorption spectra were determined surface plasmon resonances for both Au and Ag NPs. For SERS detection of nitro group compounds we used two approaches: (1) mixing those NPs with analytes in solution and (2) drop-casting with following drying of NPs on Si substrate and then drop-casting analytes on formed structure of NPs. SERS spectra were measured from both drop and dried samples in both two approaches. As nitro group compounds we investigated were the next analytes (explosive analogues): 4-nitrophenol, 1-nitronaphthalene, 5-nitroisoquinoline, picric acid - 2, 4, 6-trinitrophenol. We were able to detect all analytes with concentrations down to 10-6M both dropped on our SERS substrates and mixed with NPs.

This work was funded by grant of the NAS of Ukraine to research laboratories/groups of young scientists № 06/01-2025(5).

#### Type of presence:

Presence online

Poster Session / 153

### Perovskites with variable bandgap as the basis of new semiconductor materials

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Hybrid organic–inorganic lead-based perovskites have attracted significant attention from the scientific community over the past decade. These compounds have been successfully employed as active-layer materials in solar cells, light-emitting diodes, lasers, and photodetectors. The combination of their outstanding optical and electronic properties, together with the possibility of fabricating them from readily available precursors using simple processing techniques, makes the investigation of semiconductor materials with tunable band gaps, as well as the corresponding quantum dots, highly relevant. It is worth noting that aziridinium-based perovskites represent a rare class of 3D perovskites that are direct-bandgap semiconductors with relatively narrow band gaps. These compounds remain less explored than perovskites containing organic cations such as methylammonium or formamidinium.

In this work, a series of mixed-halide perovskites based on the aziridinium cation was synthesized. Single-crystal X-ray diffraction analysis was employed to determine the halide content and lattice parameters of each sample, as well as to examine the relationship between the perovskite composition and the halide content in the reaction mixture. The band gaps of the obtained materials ranged from 2.33 to 2.95 eV. Additionally, mixed-halide perovskite quantum dots were synthesized and investigated in the course of this study.

[1] Semenikhin, O. A.; Kucheriv, O. I.; Sacarescu, L.; Shova, S.; Gural'skiy, I. A. Quantum Dots Assembled from an Aziridinium Based Hybrid Perovskite Displaying Tunable Luminescence. Chem. Commun. 2023, 59 (24), 3566–3569.

#### Type of presence:

Presence online

**Poster Session / 182** 

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### Structural and morphological transformation of thermally reduced graphene oxide at high temperatures

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This work is devoted to the study of thermally reduced graphene oxide (TrGO) [1, 2] after exposure to high temperatures (500  $^{\circ}$ C and 700  $^{\circ}$ C). The structure and morphology of the obtained samples were investigated using X-ray diffraction and Raman spectroscopy methods.

Analysis of the results shows that heating GO to high temperatures leads to a significant deformation of the carbon planes. As a result of thermal treatment, initially "flat" carbon layers undergo non-uniform distortion due to the presence of oxygen and metal—oxygen groups on the graphene surface, as well as an increase in defect concentration. The "flat" graphene layers become corrugated, which results in the appearance of an additional set of lattice planes with an identity period of d = 5.06 Å on the X-ray diffraction pattern at 700 °C.

This structural feature makes TrGO a promising candidate as a thin nanospacer or functional layer in multilayer systems, particularly for tuning periodicity and phase conditions in X-ray and neutron supermirror structures [3].

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- [2] A. V. Dolbin et. al., Low Temp. Phys. 46, 293 (2020); https://doi.org/10.1063/10.0000701.
- [3] L. Mei et al., Optics Express, 31(18), 29768 (2023) https://doi.org/10.1364/OE.497888.

This work was partly supported by NASU (RSW of young scientist №12/04-2025) and the National Research Foundation of Ukraine (Project № 2023.03/0012).

#### Type of presence:

Presence online

**SOLARIS Synchrotron: Opportunities & Beamlines / 151** 

### Research opportunities at SOLARIS synchrotron

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SOLARIS, located in Krakow, is a third-generation synchrotron facility and the only one in Central-Eastern Europe [1]. Since its first light in 2016 and the start of user operations in 2018, it has steadily expanded its infrastructure to support a wide range of scientific applications. Currently, researchers have access to seven beamlines and two cryo-electron microscopes, enabling techniques such as ARPES, XAS, PEEM, STXM, and infrared imaging at micro- and nanoscale resolutions. These tools support investigations in materials science, chemistry, biology, and physics.

Future developments include three new beamlines—ARYA, SMAUG, and MAVKA—focused on macro-molecular structure and nanoscale chemical analysis, as well as new experimental stations (NAP-XPS and OPERANDO) for advanced spectroscopy.

This presentation will provide an overview of the SOLARIS facility, highlight its current and upcoming capabilities, and showcase selected research achievements by its user community.

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**Acknowledgements:** The work is supported under the Polish Ministry of Science and Higher Education project: "Support for research and development with the use of research infrastructure of the National Synchrotron Radiation Centre SOLARIS" under contract nr 1/SOL/2021/2.

#### References

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

#### Type of presence:

Presence online

**SOLARIS Synchrotron: Opportunities & Beamlines / 192** 

### Introducing MAVKA - Ukrainian beamline at the SOLARIS synchrotron.

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Type of presence:

**SOLARIS Synchrotron: Opportunities & Beamlines / 181** 

# PHELIX - Advance Instrument for Photoemission and Soft X-Ray Absorption studies

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The PHELIX undulator beamline is installed at the synchrotron SOLARIS [1], a third-generation light source with an electron energy of 1.5 GeV and a current of 500 mA. The beamline is designed for experiments with ultra-high vacuum Photoelectron Spectroscopy (PES) and X-ray Absorption Spectroscopy (XAS) in the soft X-ray range. In the future, Ambient Pressure X-ray Photoelectron Spectroscopy (NAP-XPS) will be available at the second branch.

The soft X-ray PES and XAS end station aims to study the electronic structure of various materials, ranging from highly ordered crystalline solids to amorphous phases like ceramics, glass, or minerals. The wide range of available techniques makes this end station a powerful and unique tool for studying very complex systems. PES experiments can be conducted using Angle Resolved Photoelectron Spectroscopy (ARPES), Circular Dichroism-ARPES, Spin-ARPES, and XPS. The SPECS PHOIBOS 225 energy analyzer with a deflector system and CMOS camera allows for collecting photoemission data with an energy resolution of 2 meV and an angular resolution of 0.1°. Absorption spectra can be obtained using Total Electron Yield (TEY), Total Fluorescence Yield (TFY), and Partial Electron Yield (PEY).

The source of the PHELIX beamline is the APPLE-II type undulator, which delivers soft X-rays with the following parameters:

- Photon energy range: 40 eV to 2000 eV (horizontally polarized light),
- Polarization: linear (horizontal and vertical), circular (left- and right-handed) and elliptical,
- Photon flux: approximately 1012 photons/s at 150 eV and around 1011 photons/s for photon energies above 600 eV,
- Beam spot size on the sample: approximately 120  $\mu$ m × 50  $\mu$ m (horizontal × vertical).

The end station includes an MBE chamber capable of evaporating Fe, Co, and Sn, with the option to install additional evaporation sources. The preparation chambers enable sample preparation in a wide temperature range from  $120~\rm K$  to  $2000~\rm K$ .

[1] Szlachetko, J., Szade, J., Beyer, E. et al. Correction to: SOLARIS National Synchrotron Radiation Centre in Krakow, Poland. Eur. Phys. J. Plus 138, 595 (2023). https://doi.org/10.1140/epjp/s13360-023-04211-x

#### Type of presence:

Presence online

Synchrotron Photoemission & X-ray Spectroscopies / 155

# Controlling Dirac–Rashba and Double Dirac Surface States in Topological Crystalline Insulator via Ultrathin Transition Metal Layers

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The band structure at the topological insulator/magnetic metal (TI/MM) interface is of great significance for realizing exotic spin-dependent phenomena and advanced spin-orbitronic devices. To investigate this interface, we employ a model system consisting of submonolayer transition metal (TM) adsorbates on the surface of a topological crystalline insulator (TCI) and examine it using the angle-resolved photoemission spectroscopy (ARPES). On the polar (111) surface, we observe the coexistence of topological surface states (TSS) and Rashba-split surface states (RSS), the latter induced by the combined effects of inversion-symmetry breaking, potential gradient, and orbital angular momentum. Our investigations demonstrate that the Rashba parameter  $(\alpha_R)$  can be tuned over a remarkably wide range of 0 to 3.5 eV ·

mathring A, depending on the type and coverage of the TM adatoms. In contrast, the nonpolar (001) surface preserves inversion symmetry, and hence no Rashba-split states emerge. Instead, surface charge imbalance induces dephasing of the wavefunctions associated with the double Dirac cones, thereby diminishing the momentum-space separation between them. These findings shed light on novel phenomena occurring at the TI/MM interface, offering a versatile platform for future spintronic and quantum devices.

#### Type of presence:

Presence online

Synchrotron Photoemission & X-ray Spectroscopies / 187

### **Looking for Topological Quantum Materials With ARPES**

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Quantum materials is a rather broad class of materials which have properties emerging from quantum mechanics and collective quantum effects, but can't be explained in classical terms (perfect example being superconductors). Non-trivial topology of their electronic structure brings in even more interesting phenomenon which can be very desired for applications such as quantum computers and spintronics. Angle-resolved photoemission spectroscopy (ARPES) with synchrotron as a light source is a perfect experimental method to study such materials as it allows to directly measure their band structure. The study of such multiband electronic structure is the key to the understanding of quantum materials and to the design of new materials with desired properties. The talk will cover a few studies of candidates for non-trivial topology including samples measured at SOLARIS.

#### Type of presence:

Presence at Taras Shevchenko National University

Synchrotron Photoemission & X-ray Spectroscopies / 190

### A ToF-PAX-RIXS Endstation for Combined ARPES and RIXS Studies at the P04 Beamline

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We report a new ToF-PAX-RIXS endstation at P04 beamline at PETRA III, Hamburg, a development of a promising novel approach to RIXS. It is based on a ToF photoemission microscope (momentum and real space imaging), allowing ARPES and RIXS studies carried out back-to-back. While RIXS is a powerful method for studying low-energy quasiparticle excitations like phonons or magnons, ARPES remains the method of choice for electron band structure investigations. Together they will help characterizing electron-phonon and electron-magnon interactions in strongly correlated material phases (Mott insulators, CDW, high-Tc superconductors).

While conventional RIXS spectrometers rely on large optical grating spectrometers, the PAX (photoelectron spectrometry for analysis of X-rays) method is based on scattered X-ray light spectrum converted into a photoelectron spectrum and can be done in a compact photoemission electron microscope. Moreover, ToF-PEEM setup offers simultaneous multichannel detection in a range of scattering angles and loss energies. In turn, acquired data is more complicated and presents essentially a convolution of two spectra: the sample's inelastic X-ray response and the photoemission spectrum of the converter foil. Reliable high-resolution deconvolution of this data is a critical step of the experiment.

As a benchmark, an undoped CaCuO<sub>2</sub> cuprate film was investigated. Existing RIXS studies have shown distinguishable phonon and magnon resonance peaks at Cu L3 edge in this system. Au, Ag and Pt converter foils have been tested for their performance, all showing promising PAX spectra, and our preliminary data evaluation managed to bring out major RIXS features.

#### Type of presence:

Presence online

#### Synchrotron Photoemission & X-ray Spectroscopies / 186

# Synchrotron VUV Study of Luminescent Properties in Mn-Doped ZnO–ZrO<sub>2</sub> Ceramics

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The luminescent behaviour of transition-metal ions strongly depends on the host lattice structure, defect concentration, and cation site occupancy. Owing to their ability to adopt multiple oxidation states, Mn ions can serve as sensitive optical probes in wide-bandgap oxide ceramics. In this work, we investigated the light-emitting properties of Mn-doped ZnO–ZrO<sub>2</sub> ceramics using synchrotron-based vacuum ultraviolet (VUV) excitation at the P66 beamline of PETRA III (DESY, Hamburg). The samples were prepared by solid-state reaction of the corresponding oxides at 1100-1500~°C for 3 h in air, with Mn concentrations of 0.01 and 0.1 at.%. Their structural and optical properties were also studied using FTIR spectroscopy, UV–Vis diffuse reflectance, SEM, and EDS analyses.

The emission–excitation maps revealed distinct luminescence behaviour depending on sintering temperature and excitation energy. Ceramics sintered at  $1100-1200~^{\circ}$ C exhibited two main components: a broad green emission excited by 250–300 nm radiation associated with ZnO-related defects, and a narrower green band excited at 150–200 nm, characteristic of ZrO<sub>2</sub>-based regions. Upon Mn incorporation, a broad orange photoluminescence band emerged, becoming more pronounced at sintering temperatures above 1300  $^{\circ}$ C, where strong densification and partial stabilization of the tetragonal ZrO<sub>2</sub> phase occur. The observed luminescence evolution is attributed to competition between Mn dopants and intrinsic defects coexisting within multiple structural phases. These findings highlight the sensitivity of Mn-related emission to local structure and demonstrate the potential of VUV excitation for probing defect- and dopant-related luminescence in complex oxide ceramics.

#### Type of presence:

Presence online

Synchrotron Photoemission & X-ray Spectroscopies / 175

### Copper site occupancy and valence in lead apatites via XAS at ASTRA/SOLARIS

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We report Cu K-edge XANES/EXAFS results on a series of Cu-substituted lead apatites Pb10-xCux(YO4)6Z (x  $\approx$  1), Y = P, V; Z = (OH)2, F2, Cl2, Br2, I2. The aim was to test the site preference and valence state of Cu in the apatite lattice, following the experiment proposed at SOLARIS/ASTRA. XANES edge positions and comparison to CuO/Cu<sub>2</sub>O standards demonstrate that Cu is unambiguously in the Cu2+ (3d9) state in all measured samples, which is the valence required by band-structure scenarios invoking flat Cu-derived bands near  $E_n$ . EXAFS fitting with FEFF-based models shows that for phosphates and vanadates with  $F_2$ ,  $Cl_2$ , and  $Br_2$  channel anions, Cu occupies predominantly the Pb(I) (4f) site, in line with our DFT site-energy hierarchy. A notable exception is found for the iodide and phosphate–hydroxyl members, where the best fits require a mixed Pb(I)/Pb(II) (4f/6h) occupation, indicating that channel size/polarizability and local OH coordination reduce the energetic penalty for Cu on Pb(II). These experimental site fractions constrain the realistic Cu distributions that should be used in electronic-structure models of Cu-Pb apatites and clarify why some compositions may fail to exhibit the predicted correlated or flat-band features. The results are in broad agreement with DFT estimates, and confirm that XAS is an effective discriminator of Cu site and valence in this materials family while.

#### Type of presence:

Presence at Taras Shevchenko National University

Workshop on Laser processing of materials for advanced optoelectronic applications / 180

# Direct optical lithography and scanning laser processing of materials for advanced optoelectronic applications

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A large number of modern micro- and optoelectronic devices and advanced sensor technologies does not require fabrication tools with ultimate resolution like a currently commercialized 2 nm technology of silicon-based chips. These are, for example, stand-alone microsensors or MEMS, for which a low price is preferred, while there is no need for close packing or miniaturization below \( \mathbb{M} \mathbb{m}\)-scale. Some applications pose even fundamental limitations on the device dimensions, for instance IR or THz sensing elements (or antennas) cannot be smaller than the targeted wavelength (which is in \( \mathbb{M} \mathbb{m}\)- or tens-of-\( \mathbb{M} \mathbb{m}\)- scale).

This situation stimulates the development of the methods and technologies for a more efficient (i) formation and characterisation of various micro-systems and (ii) controlled local modification of the material's properties at the  $\boxtimes$ m- and sub- $\boxtimes$ m- scale.

Advancement in CW and pulsed solid-state and semiconductors laser technologies enabled affordable high-quality lasers over the whole visible and near infrared spectrum. Owning to the small size and weight, then can be integrated into computer-controlled scanning system for a very fast patterning and processing of materials.

Due to these instrumental developments, the field of direct optical lithography started to grow. The use of traditional photomasks is not a sufficiently flexible method of creating device structures at the stage of their development and research, since to make even minor changes to the architecture of the device, it is necessary to produce a completely new set of masks. That is why non-contact photolithography based on laser sources are gaining more and more popularity in the research sector as a method of structuring materials and modifying their physical properties, which could be a

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new qualitative breakthrough for the entire industry in the nearest future.

Maskless photolithography is a convenient tool that allows us to create not only surface structures and mask designs, but also 3D optical structures. It has been successfully applied to structuring thin quantum dot films, production of contact electrodes for 2D materials with flake sizes of 1-2  $\mu$ m for field-effect transistors, receiving antennas of THz radiation receivers, enhancement of IR absorption by detectors, and many other applications.

The development of the maskless lithography in Ukraine for research and education purposes is initiated in the framework of the research project "Creation of a State Key Laboratory «Centre of critical optoelectronic micro-/nano-technologies and expertise»"funded by the National Research Foundation of Ukraine at the V. Lashkaryov Institute of Semiconductor Physics of the National Academy of Sciences of Ukraine.

This work was supported by NRFU project #2023.05/0022

#### Type of presence:

Presence online

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### Ultrashort Pulse Laser Microfabrication Technologies at FTMC

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Ultrashort laser pulses enable precise material processing with exceptional spatial and temporal confinement. Because the pulse duration is shorter than the electron–phonon relaxation time, the material experiences minimal or no heat-affected zone. This phenomenon underpins most of the laser–matter interaction research conducted at the FTMC Laser Microfabrication Laboratory. Our activities cover a wide range of topics, including rapid and efficient ablation, 3D engraving, GHz burst processing, laser polishing, glass micromachining (milling, cutting, scribing, welding), femtosecond laser-induced selective etching (FLICE), laser-induced periodic surface structures (LIPSS), laser coloring, surface functionalization, plasmonic sub-microstructures, and selective surface activation induced by laser (SSAIL), among others.

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### Single-Pulse Nanosecond Laser Patterning of Nanoscale Electronic– Structural Landscapes in GeSn

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GeSn alloys are promising for CMOS-compatible photonics and electronics, offering band-gap engineering from SWIR to MWIR, on-chip light sources/detectors, and strain-tunable high-mobility channels. Yet, pushing Sn content high enough for direct-gap behavior remains difficult due to low Sn solubility in Ge, growth-induced compressive strain, defect generation, and a tendency to segregate or phase separate. Laser processing emerges as a versatile, maskless post-processing route that can precisely tailor the structure and electronic properties with sub-micrometre selectivity by adjusting the pulse duration and fluence.

We investigate single-pulse nanosecond treatment of epitaxial GeSn and interrogate the response with a co-registered nanoscale toolkit: AFM for relief, SCM and KPFM for local nanoelectronics, and micro-Raman mapping for strain/composition. Nanosecond pulses generate wide heat-affected halos in which electronic reconfiguration evolves away from the crater, enabling selective modulation of carrier type, band bending, and lateral depletion correlated with Raman-resolved strain/composition fields. We establish a direct, resolved linkage between structural (strain and Sn redistribution) and electronic (surface potential, carrier type, depletion) responses in GeSn under single-shot nanosecond excitation. The treatment writes robust nanoelectronic motifs: ring-like lateral junctions at the rim, tunable depletion wells, and a low-CPD annulus co-located with resolidified edges. From these observations we outline a processing–property map for nanosecond laser post-processing, in which fluence selects electronic landscape width and contrast. This positions single-pulse nanosecond irradiation as a practical maskless route to seed lateral and vertical junctions and programmable potential profiles in GeSn devices.

The work is supported by NSF EAGER 2423217 and NRFU 2023.03/0060.

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### Laser reduction of Graphene Oxide films on SiO2-Si structures

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To form CMOS compatible graphene device the graphene oxide reduced by CW laser (455 nm) on SiO2/Si wafer was used. The graphene oxide water solution was deposited on SiO2/Si structure by drop casting method with following heating at 50°C for 1 hour. For reduction of the GrO film the laser power from 0.100 W to 0.800 W was employed, as in air and in nitrogen atmosphere. The part of samples was treated in air with additional heating at 100C. For scribing of the GrO film on SiO2 the power more than in factor 10 was used.

Analysis of electrical properties, surface morphology and structure of the laser reduced strips and comparison with thermal annealing in air at 25 ItoC for 15 minutes using correspondingly I-V characteristics, Hall effect measurements, SEM and AFM techniques and Raman spectroscopy were performed.

Raman spectra demonstrated that the laser reduction allows us to obtain graphene structure considerably better than with thermal annealing at 250C for 15 min. It is worthy noted, that relation of ID/IG lines, which determines defectivity of the material, is minimal for 0.150 W light power in case of treated at air with additional heating, for 0.550 W in case of treatment in air without heating and for about 1 W in case of treatment in nitrogen atmosphere without heating. Nature of this phenomenon is discussed and other electrical and structural characteristics obtained in the optimal regimes of the laser treatment are presented.

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### Formation and Properties of GeSn and GeSn:C Films

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Ge1-xSnx alloys are promising CMOS-compatible materials for developing effective light absorbers and emitters integrated into Si opto- and nanoelectronics. Critical to this application is the transition from an indirect- to a direct-gap semiconductor, which is experimentally observed when the Sn content is in the 6-10 % range. The wide variation in Sn values is due to the sensitivity of the material to internal deformations and the doping level. We propose two approaches to mitigate local strain: 1) incorporating carbon © atoms, which have a significantly smaller covalent radius than Sn; 2) crystallizing amorphous GeSn films using rapid thermal processing to prevent Sn segregation. To implement these ideas, GeSn films formed by thermal or magnetron deposition were co-doped with carbon. Annealing was conducted using femtosecond (fs) or scanning continuous-wave (cw) lasers. The films were characterized using Raman spectroscopy, XRD, mass spectrometry, AFM. Mass spectrometry revealed a strong correlation between the distribution of Sn and C atoms in both unannealed and annealed films. Raman analysis of the annealed GeSn films demonstrated that fs laser annealing was the most effective method, achieving a high substitutional Sn content. Importantly, the properties of films annealed using a scanning cw laser approached those of the fs laser-annealed films. Given that scanning cw laser annealing is significantly more cost-effective and simpler than fs laser processing, and more efficient than traditional thermal annealing, its application presents a highly promising and scalable path for the fabrication of high-quality, direct-gap GeSn and GeSn:C films.

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### Fabry-Pérot Enhanced THz Sensitivity of Antenna-Coupled HgCdTe Detectors

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The efficient detection of terahertz (THz) waves remains a critical challenge, despite the vast potential of the THz spectrum. We present a method to significantly enhance the sensitivity of THz detectors featuring a metallic antenna on a conducting film with a dielectric substrate. The study utilizes mercury-cadmium-telluride (HgCdTe), a proven semiconductor for infrared detection, extending its capabilities into the THz range.

Our approach proposes leveraging the Fabry–Pérot (FP) interference effect to maximize the electromagnetic (EM) energy absorbed within the conducting film by precisely adjusting the substrate thickness. We modeled and fabricated THz detectors consisting of a bow-tie antenna on a p-type HgCdTe film with a CdZnTe substrate. Electrodynamic modeling and simulations, focusing on the 140 GHz frequency, revealed that the EM energy oscillates dramatically as a function of substrate thickness. Simulations predicted that average field intensity in the film could be enlarged by using the optimal substrate's thickness.

Experimental results comparing samples with near-optimal and non-optimal CdZnTe substrate thicknesses confirmed the theoretical predictions. The optimization strategy yielded more than a three-fold increase in sensitivity (an enhancement factor of approximately 3.2 in photoresponse: 3.63 nA vs 1.14 nA). This technique provides a practical and effective way to significantly improve the sensitivity of single-frequency or narrow-band THz detectors without requiring complex fabrication changes or cryogenic cooling systems. Furthermore, this substrate optimization method is compatible with established semiconductor manufacturing processes, suggesting potential for integrated dual-band IR-THz systems based on the HgCdTe platform.

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# Photoinduced formation of semiconductor nanocrystals in amorphous arsenic chalcogenides

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Amorphous arsenic chalcogenides are semiconductor materials known for numerous photoinduced effects under illumination by light of appropriate energy and intensity which makes them promising for various applications. We present a study of photoinduced formation of semiconductor nanocrystals in amorphous As–S(Se) films doped with metal atoms. The doped As2S3 and As2Se3 films with desired dopant content were prepared by thermal evaporation on silicon and silicate glass substrates. The prepared samples were of small surface roughness, however, as confirmed by the X-ray photoelectron spectroscopy data, the dopant content noticeably decreased with the film depth.

Raman spectroscopy (Horiba LabRAM HR 800 or Horiba XPloRa Plus) was a technique to provide the light of appropriated energy and intensity, and simultaneously an in situ means of detection of the photoinduced changes in the material.

Frequencies of relatively sharp peaks that emerge in the Raman spectra of doped amorphous arsenic chalcogenide films at sufficient laser power densities correspond to phonons of nanocrystals formed on the film surface with the participation of the dopant atoms, e. g. CdS in As2S3:Cd, CdSe in As2S3:Cd, ZnS in As2S3:Zn, etc. Laser-induced photosoftening of the amorphous arsenic chalcogenide films and enhanced diffusion result in energetically favourable formation of nanocrystals in

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the laser spot. The presence of nanocrystals is verified by Raman and photoluminescence (PL) spectroscopy. Raman spectroscopy can provide accurate identification of the nanocrystals formed in the amorphous As2Se3-based matrix under illumination while PL is a more sensitive technique to detect their presence in the sample.

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