

**The 1st Serbian Conference on Materials Application and Technology - SCOM**

**BOOK OF ABSTRACTS**

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# **SCOM 2022**

**The 1st Serbian Conference on Materials  
Application and Technology**

**BOOK OF ABSTRACTS**

Belgrade, Serbia, 20<sup>th</sup> - 21<sup>st</sup> of October 2022

Dear Colleagues and Friends,

It is our great pleasure to welcome you to the first Serbian Conference on Materials Application and Technology - SCOM2022. The conference is jointly organized by the Society for Science Development of Serbia and the Vlatacom Research and Development Institute. With a focus on cutting-edge materials design, fabrication, and integration as well as ground-breaking materials-based technologies, SCOM2022 is the new home for all materials-related technological research. This conference will highlight the most recent advancements in the field of materials technology and application aiming to bridge the gap between researchers working on materials and technology users. Energy, healthcare, electronics, optics, microfluidics, sensors, food safety, and other topics will be covered. This year, three tutorial lectures, two invited lectures, and 16 oral presentations on the following topics will be given: Nanomaterials, Biomaterials, Optical and Photonic Materials, Materials for energy production and storage, Chemo/Bio/Physical Engineering, Photocatalysis, Green technologies, Sensor materials and technologies, Materials synthesis and processing.

We anticipate that SCOM2022 will be fruitful in terms of scientific exchange and that it will strengthen existing collaborations among participants while also fostering future ones. We would like to thank various organizations for their financial assistance.

Organizers of the SCOM2022 wish you a nice time during the conference in Belgrade!

Conference Chairperson

Prof. Dr. Miroslav D. Dramićanin

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## RARE EARTH DOPED CRYSTALS FOR QUANTUM TECHNOLOGIES

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*Keywords:* quantum technologies, rare earth, coherent spectroscopy

Systems with both spin and optical transitions offer a range of functionalities for quantum technologies [1]. They allow storage and entanglement of photonic quantum states for quantum communications, interfacing processing nodes with optical networks for distributed quantum computing, or efficient detection for quantum sensing. Among various solid-state systems currently considered, rare earth doped materials stand out as they combine, at cryogenic temperatures, long-lived optical and spin quantum states [2]. In addition, they offer optical transition in a wide spectral range, including telecom wavelengths, high chemical stability, and easy doping in many hosts, thus enabling using large ensembles of centers with uniform properties.

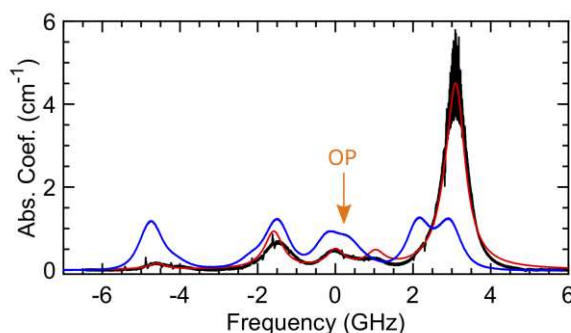


Fig. 1. Diffusion enhanced optical pumping (DEOP) in  $171\text{Yb}^{3+}:\text{Y}_2\text{SiO}_5$  [3]. After Yb optical pumping (OP) at a fixed frequency, a drastic change in the absorption spectrum (blue to red line) is observed as  $>96\%$  of spins are polarized to a single hyperfine ground state level (red line).

Quantum-grade rare earth doped materials are developed in different forms. They include bulk crystals, like  $\text{Y}_2\text{SiO}_5$ , in which exciting demonstrations have been performed, and more recently nanostructured materials such as nanoparticles or thin films, aiming at integration into nanophotonics devices. New platforms and approaches are also studied, taking advantage of ion implantation, molecular chemistry or hybrid structures for example. This fast-expanding field has witnessed impressive progress and hold exciting promises for a broad range of quantum-based applications. In this tutorial, we will review the most important features of rare earth doped crystals for applications in this field, as well as recent advances and current challenges

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## **Molecular Recognition Using Nanomechanical Photothermal Spectroscopy**

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Resonant optical excitation of targeted molecules provides very high spectroscopic selectivity in chemical and biomolecular detection. Although radiative relaxation is often used for chemical and biological sensing, obtaining high sensitivity and selectivity in detection requires complex and bulky equipment. However, non-radiative relaxation of resonantly excited molecules, that can generate extremely small amounts of heat by photothermal effect, can be detected using microfabricated cantilevers. Cantilevers, when fabricated as bi-material beams, have a thermal sensitivity in the milli Kelvin range at ambient temperature. In addition to photothermal signatures of adsorbed molecules, micromechanical resonators can also provide adsorbed mass and adsorption energy with a very high sensitivity. These cantilever resonators can also be fabricated as microfluidic channels for characterizing confined or flowing liquid samples in them. This approach provides a label-free and receptor-free method for molecular recognition, and overcomes many of the selectivity challenges encountered when using receptor-based approaches. Understanding energy dissipation at resonance can impart additional information for enhancing the selectivity. Multi-modal, multi-physics data obtained with the nanomechanical platform, when analyzed using deep learning techniques, can enhance the selectivity, sensitivity, and reliability even in complex mixtures and environments.

## **Electron Paramagnetic Resonance as a unique and powerful tool for point defects study. Application in various branches of science and industry**

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For better clarity, the basics of EPR will be given to determine the place of this method in the family of techniques dedicated to the new materials engineering. EPR is applicable to the paramagnetic systems, i.e., the particles having at least one unpaired electron (uncompensated electron spin) in the outer shell. In particular, it is exceedingly useful for the point defects study, either external or internal ones. The external defects can be intentional, used for the material doping in order to gain specific properties or unintentional, appearing in the material either from precursors or crucible. Charge state, local structure, distribution and incorporation of the defect as well as its influence on the optical or electric properties can be determined. Therefore, the feedback to the technology can be given. Another exceedingly useful ability of the EPR technique is the internal defects investigation. These are typically vacancies and interstitials. Vacancies can trap charge carriers. Moreover, charge carriers can be trapped at regular or substitutional ions. It should be noted that EPR is one of the powerful techniques, much more sensitive than X-ray diffraction, X-ray fluorescence, X-ray photoelectron spectroscopy. Moreover, each paramagnetic point defect has its typical “visit card” which leads to the precise determination of its origin. Note, that EPR can be applied to the paramagnetic particles concentration determination.

The typical objects of the investigation can be inorganic (ions and other charged particles) as well as organic substances (radicals, lipids, proteins, living tissues and cells) appearing in the form of single crystals, polycrystalline bodies, powders, ceramics, glasses, liquids, gases etc. The objects can also be micro- to nanoscale, including quantum dots. Moreover, the effect of ionizing radiation can be studied both in inorganic and organic matter as well. Therefore, EPR has the potential to solve different tasks appearing in many branches of the applied science and industry. These include Physics, Chemistry, Biology, Medicine, Pharmacology, Material Sciences, Environmental sciences and Ecology as well as Food control. Application of EPR in combination with other methods and techniques provides exhausted information about the objects of study. Practical examples are given.

## **Mn<sup>4+</sup>-DOPED K<sub>2</sub>TiF<sub>6</sub> RED-EMITTING COMPONENT FOR MODERN WHITE LEDs**

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Although the traditional co-precipitation method is widely used to produce several types of hexafluoride red-emitting phosphors, their photoluminescence quantum efficiency is insufficient for white LEDs. A novel organic solvent-assisted co-precipitation method, on the other hand, is used to prepare highly efficient Mn<sup>4+</sup>-doped K<sub>2</sub>TiF<sub>6</sub> red-emitting phosphor. The phosphor particle size was controlled by using organic solvents with an alcohol functional group and different carbon chain lengths in the synthesis. The synergistic effect of the organic solvent and hydrofluoric acid leads in large smoothed hexagonal-shaped crystal sheets of particles that become larger as the carbon chain length of organic solvent increases. The excitation photoluminescence spectra show two broad excitation bands originate from the spin-allowed transitions of  ${}^4A_{2g} \rightarrow {}^4T_{1g}$  and  ${}^4A_{2g} \rightarrow {}^4T_{2g}$ . The blue excitation band (420 – 520 nm) is stronger than the UV band (320 – 410 nm), suggesting that K<sub>2</sub>TiF<sub>6</sub>:Mn is suitable for white LEDs based on a semiconductor blue chip. Under 466 nm excitation, the emission photoluminescence spectra of K<sub>2</sub>TiF<sub>6</sub>:Mn consists of typical sharp red Mn<sup>4+</sup> emissions in the 595 – 660 nm wavelength range. The photoluminescence properties of K<sub>2</sub>TiF<sub>6</sub>:Mn strongly depend on the size and thickness of particles. The addition of n-butanol during the synthesis of K<sub>2</sub>TiF<sub>6</sub>:Mn increases the intensity of strong and sharp emission at 628 nm by 208%. The lifetime of Mn<sup>4+</sup> ( ${}^2E_g \rightarrow {}^4A_2$  transition) in non-organic solvent prepared K<sub>2</sub>TiF<sub>6</sub>:Mn was estimated to be 5.65 ms, whereas the lifetime values of phosphors prepared by organic solvent-assisted synthesis were higher due to the less efficient non-radiative processes. The photoluminescence quantum efficiency of phosphors prepared using an n-butanol-assisted co-precipitation method is very high (98.2%), much higher than that of the same phosphors prepared using the traditional co-precipitation method (89.9%). Our findings reveal a new method for producing K<sub>2</sub>TiF<sub>6</sub>:Mn phosphors with controlled morphology and very high quantum efficiency, as well as a simple strategy for optimizing all Mn<sup>4+</sup>-activated hexafluoride phosphors that are highly desirable in white LEDs.

## Silver-Bismuth Iodide Rudorffites as Light Absorbers in Photovoltaic Devices

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### Abstract:

Silver-bismuth iodide (Ag-Bi-I) rudorffites are chemically stable and non-toxic materials that can act as a possible replacement for methylammonium lead halide perovskites in optoelectronic devices. In this report we will present innovative routes for fabrication of Ag-Bi-I nanomaterials, as well as the results of the investigation of the electronic structure of isolated Ag-Bi-I nanoparticles by soft X-ray aerosol photoemission spectroscopy [1, 2]. Aerosol photoemission spectroscopy allows studies of the electronic structure of submicrometer particles that are free from the influence of a substrate or solvent [1-5]. In this approach, the aerosol particles can be produced directly from a solution or a colloidal dispersion, which opens a possibility for investigation of a variety of nanosystems that can be produced by wet chemistry methods. This technique relies on the interaction of focused beam of isolated particles with ionizing radiation under high vacuum conditions. In addition, by using tunable synchrotron radiation as an excitation source it is possible to obtain high-resolution photoelectron spectra in the investigated photoelectron energy range.

Keywords: lead-free perovskite, silver-bismuth iodide, electronic structure, photoemission spectroscopy

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# NUMERICAL SIMULATION OF TITANIUM ALLOY HIP IMPLANTS BEHAVIOUR UNDER STATIC AND DYNAMICS LOADS

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This paper presents the development of numerical models for simulation of behavior of titanium alloy hip implants under static and dynamics loads, which is a part of an extensive research involving the structural integrity of such implants under various loading conditions, such as fatigue and corrosion. Numerical models were made in both ABAQUS and ANSYS software packages, in order to determine the stress/strain distribution and the number of cycles and stress intensity factors, for two different hip implant geometries. The next stage of this analysis involved comparing these two cases, in order to determine which, one has better behavior, depending on the exploitation conditions, which can vary greatly between different groups of patients. For this purpose, failure assessment diagrams were made for both geometries, assuming the crack length of 1 mm.

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## OPTIMIZATION OF THE EXTRACTION PROCESS FROM *SATUREJA MONTANA* L.: PHYSICOCHEMICAL CHARACTERIZATION OF THE EXTRACTS

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Winter savory (*Satureja montana* L.) is a widely known medicinal plant species, which has been cultivated from seeds at the experimental field of the Institute “Dr Josif Pančić”, Pančevo, Serbia. The plant material used in this study was harvested from a 6-year-old plant. The aim of the study was to optimize the standard maceration process for polyphenol extraction from air-dried plant material, utilizing 50% ethyl alcohol solution. The optimization was performed through varying two most important parameters for maceration: solid-to-solvent ratio and extraction time. The obtained extracts were characterized *via* analyzing the total polyphenol content (TPC), total flavonoid content (TFC), antioxidant potential (ABTS, DPPH, FRAP, and CUPRAC assays), extraction yield, conductivity, density, surface tension, and viscosity. The TPC varied from  $7.15 \pm 0.8$  to  $92.2 \pm 2.5$  mg gallic acid equivalent (GAE)/g of plant material. Further, the extraction time and solid-to-solvent ratio had significant influence on TFC; the highest values were achieved between 30 and 90 min, and at a 1:40 ratio. The highest ABTS<sup>•+</sup> and DPPH<sup>•</sup> radical scavenging activities were detected in the extracts prepared using 1:30-1:50 ratios, while the best ferric and cupric ion reducing antioxidant potential was measured in the extract obtained at a 1:50 ratio. The highest extraction yield was detected in the extract obtained at a 1:50 ratio ( $86.0 \pm 2.9\%$ ), whereas the extraction time did not have a statistically significant influence on the mentioned parameter. On the other hand, the highest value of conductivity was measured in the extract prepared at a 1:10 ratio, and the highest density and surface tension of the extract was obtained at a ratio of 1:40 ( $0.941 \pm 0.002$  g/mL and  $29.0 \pm 0.1$  mN/m, respectively), while the highest viscosity was measured in the extract prepared at a 1:20 ratio ( $2.89 \pm 0.02$  mPa·s). In the present study, the optimization of the extraction was performed, in specific, the extraction time and solid-to-solvent ratio levels for improving the efficiency of polyphenols extraction from *S. montana* were determined. Our study shows the possibilities for production of polyphenols-rich extract of *S. montana* which might be used in pharmaceutical, food or cosmetic products.

## PHONON INVESTIGATION IN $\text{YVO}_4:\text{Eu}^{3+}$ NANOPOWDERS

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In this paper two methods of preparation of yttrium orthovanadate nanopowder were presented: top – down approach, Solid State Reaction and bottom – up approach, Solution Combustion Synthesis.

We report the change in reflection spectra in europium doped  $\text{YVO}_4$  nanopowders with comparison to its bulk analog. In UV – Vis reflection spectra we consider the change in values of band gap in these structures, after resizing it from bulk to nanomaterial. We show the existence of Surface Optical Phonon (SOP) and different phonon processes which alter the reflection spectra of bulk  $\text{YVO}_4$ . Reflection IR spectra were modeled using classical oscillator model with Drude part added which takes into account the free carrier contribution. Since our materials are distinctively inhomogeneous materials, we use Effective Medium theory in Maxwell Garnett approximation to model its effective dielectric function.

For full structural characterization, X – Ray Powder Diffraction and Field Emission Scanning Electron Microscopy were used.

## CHANGES IN SAMPLES CHARACTERISTICS DUE TO LASER POWER

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The phase changes of two different types of nanoparticles, ZnO(Co) and MnO, under laser power have been studied. Nanocrystalline samples of ZnO(Co) prepared by commonly used wet chemistry method followed by calcinations was investigated first, while MnO nanoparticles, purchased from Sigma-Aldrich Co., were investigated next. Previous confirmation of the existence of ZnO and Co<sub>3</sub>O<sub>4</sub> phases in ZnO(Co) and MnO phase in MnO were based on the X-ray diffraction measurements. Here we report the experimental spectra of non-resonant Raman scattering in the range between 100 cm<sup>-1</sup> and 1600 cm<sup>-1</sup>, for both type of samples and far-infrared spectroscopy (FIR) at room temperature, in spectral region between 80 and 660 cm<sup>-1</sup> for MnO sample. A series of ZnO(Co) samples were irradiated with four different laser power densities, while MnO sample was irradiated with eight different laser powers.

We notice that the laser power has different influence on relative intensity of peaks that belong to ZnO phase than on those corresponding to Co<sub>3</sub>O<sub>4</sub> phase in ZnO(Co) samples. Both peak types show characteristic broadening and red shift toward lower frequencies. The laser power densities used in our study did not cause thermal destruction in any of the investigated samples. Laser-induced local heating effects in samples caused formation of cobalt dimers on the surface of Co<sub>3</sub>O<sub>4</sub>.

The laser power has produced change in existing phases in MnO sample, destruction of MnO phase and creation of MnO<sub>2</sub>, Mn<sub>3</sub>O<sub>4</sub> and MnOOH phases along with formation of Mn<sup>2+</sup> on the sample surface. These phase changes has been confirmed by X-ray diffraction and AFM measurements for Raman study. The FIR spectra were analyzed by using Maxwell-Garnet formula, where MnO nanoparticles are modeled as a mixture of homogeneous spherical inclusions in air. Laser power leads to the conversion of the part of MnO nanoparticles into the MnO<sub>2</sub>, Mn<sub>3</sub>O<sub>4</sub> and MnOOH, along with possible formation of elemental MnO on the sample surface.

Does calcinations temperature change behavior of sample under laser power and how? That is a goal of our future investigation.

## **The development of composite hydrogels based on poly(methacrylic acid), natural polymers and nano-structured particles of calcium phosphate ceramics for biomedical applications**

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Hydrogels are three-dimensional hydrophilic networks of polymers capable of retaining large amounts of water or biological fluids. A highly hydrated, porous structure of hydrogels resembles the structure of living tissues, making them particularly attractive for a wide range of biomedical and pharmaceutical applications. Various types of synthetic and natural polymers have been investigated as hydrogels for biomedical purposes. Amongst them, poly(methacrylic acid) (PMAA) hydrogels have gained increased attention in the field of biomedicine due to pH-triggered swelling, tunable porosity and mechanical properties, biocompatibility, etc. However, pristine PMAA hydrogels do not meet all requirements for biomedical applications, such as biodegradability, cell activity promotion, high mechanical strength and controllable drug release kinetics, which requires thought-provoking strategies to improve the properties of the hydrogels. Over the last years, remarkable progress in the properties of hydrogels has been achieved by developing interpenetrating network hydrogels (IPN) based on different types of strengthening mechanisms, as well as incorporating different inorganic particles into a polymeric matrix. In this work, we present the results of our research on PMAA-based hydrogels for potential biomedical applications. The main focus of the research was the synthesis of IPN of PMAA and different natural polymers, as well as the incorporation of nano-structured particles of calcium phosphate ceramics. The obtained materials were evaluated in terms of mechanical properties, porosity, swelling ability and drug deliverability.

## OPTICAL NANOSOURCES BASED ON TUNNEL TRANSITION CREATED BY THE STM NANOLITHOGRAPHY

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The optical interconnection between parts of the integrated circuits and, for example, between the CPUs and memory is the good way to improve the performance of computing systems[1,2]. But for realizing of this idea, the optical light sources must have similar sizes as modern semiconductor components.

One of the approaches to realize such photon or surface plasmon-polariton (SPP) source is the use of light emitted tunnel junction (TJ) [3]. Local TJ contact is small (defined by the size of contacts), ultra-fast (quantum-mechanical process), does not need resonators such as in lasers, and is potentially easy to be implemented in modern integrated circuits. Unfortunately, a common tunnel junction has quantum efficiency about  $10^{-5}$ - $10^{-6}$  photons per electron. The quantum efficiency can be improved by bringing nanoantenna in the tunnel junction region[4,5].

We developed a precision technique of nanoantennas formation by voltage pulse for amplification of tunnel junction light emission. This technique is applied in ultra-high vacuum of the scanning tunneling microscope on a layered sample of a thick metal film covered with a thin silicon layer. Typical sizes of these nanoantennas start from 30 nm. The estimated emission increase is about 13 times compared to a pure gold film.

This technique allows forming the arrays of nanosized light sources which can be used for high density multichannel electrically-driven optical interconnection.

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## **WOOD AS AN ENERGY MATERIAL: MEETING ENERGY NEEDS IN THE EU-27 BY IMPORTING CERTAIN WOOD FUELS**

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**Abstract:** For decades, EU-27 countries have been investing significant efforts and funding to increase energy production from renewable sources. The implementation of this policy created the conditions for changing the structure of the EU-27 energy balance, which is dominated by fossil fuels, as well as the conditions for reducing its energy dependence. Natural persons and legal entities who wanted to use renewable energy sources were supported by subsidies. These measures have particularly contributed to the expansion of the use of wood fuels such as wood chips, briquettes and pellets. To meet the needs of its own market, the EU-27 imports significant amounts of these three types of fuels. The aim of this research was to identify the volume of imports of wood pellets, chips and briquettes in the EU-27 during the period 2010-2021. The analysis of imports of the mentioned types of fuel did not include the imports among EU members, but only from other countries of the world. This choice was made in accordance with the goal of the research, i.e. identifying the percentage of energy needs that the EU-27 met by importing the above wood fuels from other countries of the world during the period 2010-2021. Based on the obtained data, different scenarios of fossil fuels substitution with wood fuels, which occurred in the European market, were analysed. The EU-27 countries that are the biggest importers of these types of fuel have been identified, as well as the most significant countries supplying the mentioned types of fuel to the European market. The impact of the import of wood pellets, chips and briquettes on final energy consumption in the EU-27 was investigated by creating multiple econometric models. Since sustainable energy supplies are a burning issue, future research needs to analyse the types of wood biomass that are used for the production of these types of fuel. According to the second, third and fourth parts of the ISO 17225:2021 standard, wood pellets, briquettes and chips can be produced from forest, plantation and other virgin wood (biomass class 1.1. in Table 1 of the specified standard), as well as from byproducts and residues from the wood processing industry (biomass class 1.2), but also from chemically untreated used wood (biomass class 1.3.1.). In order to reduce the constantly growing strong pressure on the first type of biomass, further research should pay special attention to the calculation of volume of available biomass of categories 1.2. and 1.3.1. for the production of the three analysed types of wood fuels.

**Key words:** wood fuels, EU-27, import, final energy consumption.

## SMART TEXTILE AGAINST PATHOGENS' ATTACK

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The actual and global problem is spreading infections by pathogenic microorganisms, especially in hospitals. The Covid-19 pandemic we are facing has increased awareness of enhanced product sterility measures, all to fight pathogenic microorganisms. Also, due to the uncontrolled use of antibiotics, microorganisms have become more and more resistant to various antimicrobial agents known up to now. Fabrics, gauze, bandages, and cotton wool could absorb a high amount of moisture making this fiber more prone to microbial attack. Under certain conditions of humidity and temperature, cotton may act as a nutrient, becoming a suitable medium for bacterial growth. Although, silver in the form of ions and nanoparticles has been tested for many years and is increasingly frequent use in the production of various products for various purposes.

This study aimed to examine the antimicrobial efficiency of cotton fabrics like gauze, sanitary pads, cotton wool, compress, and bandages loaded with commercial colloidal silver (Colloid company). The influence of silver concentration and the amount of silver deposited onto the fabric on antimicrobial activity against Gram-negative bacterium *Escherichia coli* and *Pseudomonas aeruginosa* Gram-positive bacterium *Staphylococcus aureus*, *Bacillus subtilis*, and *Enterococcus faecalis*, and the fungus *Candida albicans* were studied.

The microbial reduction of the tested materials loaded with a silver solution of 30 ppm (15-20 µg of Ag on 1 g of fabric) against the Gram-negative bacteria *E. coli* and *P. aeruginosa* is almost maximum after two hours of contact, 95% and 99% of reduction, respectively. In the case of Gram-positive bacteria *S. aureus*, *B. subtilis*, and *E. faecalis*, a longer time is needed for the complete bacterial killing (over 99%), except for *B. subtilis*, where two hours of contact is sufficient for the maximum reduction of the initial number of bacteria. The microbial reduction of *S. aureus* after two hours of contact is satisfactory, but after 24 hours of contact, it is already maximal. Antifungal activity testing against the fungus *C. albicans* gave moderate antifungal activity results. After two hours of contact, there is no antifungal activity, while after 24 h there is a certain reduction in the number of microorganisms that survived, but it is not complete. We must emphasize that *C. albicans* is a representative of eukaryotic cells and results indicate that investigated materials would not be toxic to human cells.



## PREDICTION OF THERMAL AND MECHANICAL PROPERTIES OF THE ACRYLATE-BASED COMPOSITES USING ARTIFICIAL NEURAL NETWORK MODEL

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### Abstract

The role of nano-sized alumina on fracture mechanism and deformation of Poly (methyl methacrylate) (PMMA) was investigated. PMMA has a broad spectrum of uses especially in medical applications. The composites were made of PMMA modified with dimethyl itaconate (DMI) as a matrix. As reinforcement were used alumina particles ( $\text{Al}_2\text{O}_3$ ) and alumina doped with iron oxide ( $\text{Al}_2\text{O}_3\text{-Fe}$ ) modified with 3-aminopropyl-trimethoxylane (AM) and flax oil fatty acid methyl esters (biodiesel – BD). According to the thermal conductivity measurements, the highest thermal conductivity values had the composite with alumina particles with the highest alpha phase content. With the addition of modified alumina particles to PMMA/DMI matrix mechanical properties were improved (tensile strength, modulus of elasticity and elongation at break). In the current research, an artificial neural network model of acrylate-based composite combined with alumina-based particles, based on the Broyden-Fletcher-Goldfarb-Shanno iterative algorithm was investigated, for the prediction of thermal conductivity, tensile force, elongation percentage and modulus of elasticity based on the water content, Fe content and additives. It has been shown that these mathematical models can predict the mechanical and thermal properties of composite materials. This especially refers to the prediction of the thermal conductivity of materials used in dentistry for the production of dentures and which are exposed to variations in temperature during exploration.

**Key words:** composite materials; fracture; thermal properties;  $\text{Al}_2\text{O}_3$  particles; mathematical modelling.

## All near-infrared luminescent lifetime-based thermometry with $\text{Mn}^{5+}$ activated $(\text{Ba}_x\text{Sr}_{1-x})_3(\text{PO}_4)_2$ phosphors

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Here we present the near-infrared lifetime-based luminescence thermometry probes based on the  $\text{Mn}^{5+}$  activated  $(\text{Ba}_x\text{Sr}_{1-x})_3(\text{PO}_4)_2$  ( $0 \leq x \leq 1$ ) phosphors. These phosphors were prepared by solid-state method and the pure-phase rhombohedral structure is confirmed by the X-ray diffraction analysis indicating effective incorporation of dopant  $\text{Mn}^{5+}$  ions. Broad and strong absorption between 650 nm and 950 nm covering the first biological transparency window and having the absorption maximum at  $\sim 660$  nm was detected by diffuse reflectance measurements. By varying  $x$  (Ba to Sr molar content) following changes in the photoluminescent properties were observed: i) the blue-shift of the emission maximum (1191 nm  $\rightarrow$  1173 nm) (Fig. 1a) and ii) the increase in the excited state lifetime (Fig. 1b). Lifetime-based luminescence thermometry was performed on all samples and revealed relative sensitivity of  $0.5 \text{ \%K}^{-1}$  at 310 K (physiologically relevant range) and maximal value of  $\sim 1 \text{ \%K}^{-1}$  at temperatures between 400 K and 500 K. No significant influence of the cation content on thermometric properties was observed.

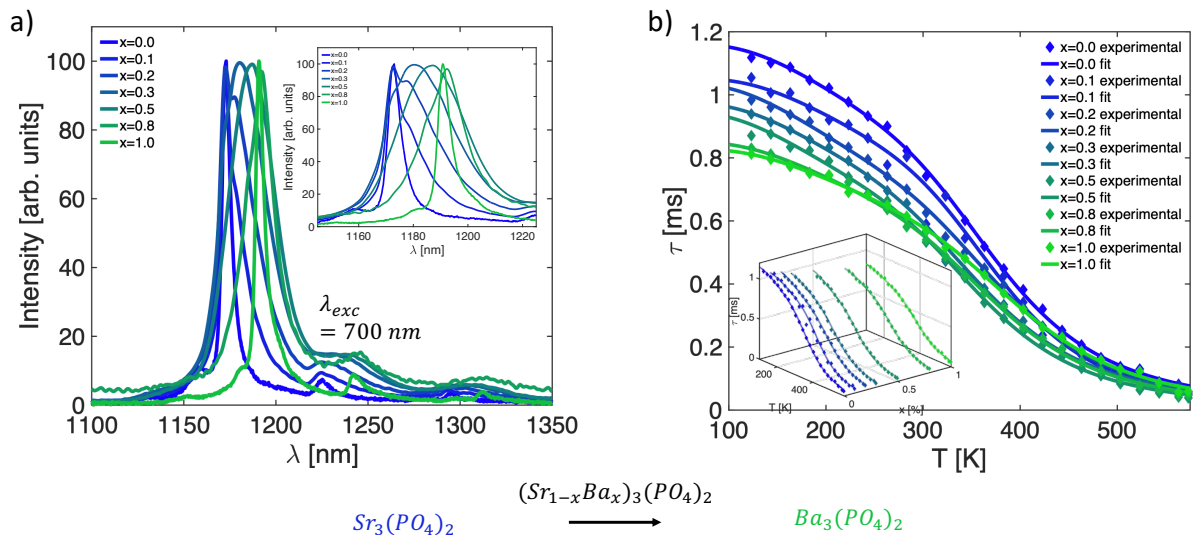


Figure 1. a) Blue shift of  $(\text{Ba}_x\text{Sr}_{1-x})_3(\text{PO}_4)_2$  luminescence peak position with the Ba content -  $x$  increasing; b) lifetime measurements as a function of both the Ba content -  $x$  and the temperature -  $T$

## Temperature invariant luminescence manometer based on Cr<sup>3+</sup> emission in Li<sub>2</sub>Mg<sub>3</sub>TiO<sub>6</sub>

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Luminescent manometers have recently been gaining more and more interest due to the need for simple non-contact pressure controlling, especially in the biomedical field, for example determining glucose concentration in blood, based on a value of osmotic pressure in cells [1]. The most widely used approach in luminescence manometry is a readout based on the spectral shift of the emission band [2]. However, it is important to note that this approach has significant limitations – when pressure readout is based on a narrow emission band, the sensitivities achieved are relative low due to the slight spectral shift, while using a broadband emission, the reading precision is limited due to an error in peak centroid determination.

Therefore, we developed a manometer that met all the challenges posed above – Li<sub>2</sub>Mg<sub>3</sub>TiO<sub>6</sub>:Cr<sup>3+</sup>[3]. A ratiometric approach (luminescence intensity ratio) on the broad emission band associated with the <sup>4</sup>T<sub>2</sub>→<sup>4</sup>A<sub>2</sub> transition of Cr<sup>3+</sup> was used. This approach allowed to minimize pressure reading error, while obtain a high relative sensitivity S<sub>R</sub> of 4.6%/GPa. In addition, the pressure readout was proven to be independent of temperature in the range of 123-563 K. On the basis of Raman spectroscopy (0-10 GPa) and cyclic emission measurements during compression and decompression, it was proven that spectral changes observed under applied pressure are reversible, which makes the proposed manometer gain high application potential.

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## SCIENTIFIC SOFTWARE FOR LUMINESCENCE BY OMAS GROUP

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Luminescent materials, simply called phosphors, are used in multi-billion-dollar industries of LEDs, displays, fluorescent lamps, lasers and optical sensors. Our group OMAS which is an abbreviation for Optical Materials and Spectroscopy investigates the fundamental properties of phosphors and their applicability for LEDs, lasers, and temperature sensing.

Temperature causes changes in all spectral features of phosphors. If the activator ion in phosphor material is a lanthanide, then intensities, quantum efficiencies and radiative lifetimes can be theoretically predicted by the Judd-Ofelt theory. By using theoretical models of temperature-dependent spectral characteristics and Judd-Ofelt theory, one can predict, simulate, and explain the properties of the phosphor light emission. However, there are numerous models and equations that may differ among various materials. Thus, doing the above-mentioned task manually is cumbersome to say at least, and in some cases even impossible. The scientific and industrial progress in modern times greatly relies on collaboration with IT, which is also the path the OMAS group undertook as a solution to this problem. For every computationally difficult task the OMAS group encountered in research, the specialized software is built to help resolve it, and the solution was always shared with other researchers in a form of publications, data shares, and via [www.omasgroup.org](http://www.omasgroup.org). All the software that was developed by the OMAS group will be presented here.

LumTHools is the most recently published stand-alone desktop application for modelling the temperature-dependent phenomena in luminescence and luminescence thermometry. It fits the experimental data to one of the many theoretical functions and provides the needed physical parameters and figures of merit. It was built in python and Java. OMAS used Mathematica and MATLAB for many functions and applets. So far these small applications are capable of modelling temperature dependence of  $\text{Mn}^{4+}$  emission decay and application to the luminescence thermometry, interactive simulation and evaluation of the performances of the sensor probe by the luminescence intensity ratio method and Judd-Ofelt theory, predicting the phosphor emission colour by  $\text{Eu}^{3+}$  spectrum simulation from the Judd-Ofelt theory, and software for deconvolution of overlapping peaks of transition metals at multiple temperatures. To be able to apply the Judd-Ofelt theory for spectroscopic analysis, it is necessary first to obtain the 3 Judd-Ofelt parameters. This is done from a single spectrum, but various methods are depending on the investigated lanthanide ion. We have published PHP calculators of the Judd-Ofelt parameters on the OMAS group website for parametrization from the excitation spectrum of  $\text{Eu}^{3+}$  and the emission spectrum of  $\text{Pr}^{3+}$ . JOES is a stand-alone desktop Java application for complete Judd-Ofelt analysis from the emission spectrum of  $\text{Eu}^{3+}$ . OMAS group also programmed ATMEL microcontrollers for various tasks: for control of LEDs to obtain the desired spectrum or for heating/cooling stages.

OMAS group over the course of several years published many, multiplatform, open source, free software using python, Java, PHP, Mathematica, C++ or MATLAB, for applications in luminescence analysis, thermometry, simulations or control of electronics. The software was published in prestigious journals and rewarded with a high number of citations.

## MICROWAVE-ASSISTED HYDROTHERMAL SYNTHESIS OF Eu<sup>3+</sup>-DOPED CsY<sub>2</sub>F<sub>7</sub> NANOPHOSPHOR

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Microwave-assisted hydrothermal synthesis is a simple and straightforward method to make lanthanide-doped luminescent nanomaterials. It combines the use of microwaves as a heating source with a hydrothermal closed reaction system. During the reaction, solvents/reactants interact with microwave radiation, resulting in rapid heating and small temperature gradients inside the reaction vessel. Different system properties, such as polarity and solvent choice, pH and volume of mixture, pressure, time, and temperature of reaction, can be used to promote the formation of targeted structures and morphologies.

CsY<sub>2</sub>F<sub>7</sub> belongs to a growing group of rare earth fluoride nanomaterials. In this case, the Y<sup>3+</sup> ion can undergo isostructural exchange with various trivalent rare earths, opening the door to a variety of luminous characteristics. The trivalent europium ion (Eu<sup>3+</sup>) is well known for its strong luminescence in the orange/red spectral region.

A novel synthetic route for Eu<sup>3+</sup> doped CsY<sub>2</sub>F<sub>7</sub> is successfully developed using microwave-assisted hydrothermal synthesis. Yttrium acetate, caesium fluoride, europium nitrate, and ammonium fluoride were used as precursors. An excess of ammonium fluoride was used to boost the reaction to the desired stoichiometry. The solution was heated to 160°C for one hour in a SiC hydrothermal vessel. The obtained nanopowder was washed and dried in air.

CsY<sub>2</sub>F<sub>7</sub>: 4%Eu<sup>3+</sup> crystallizes in orthorhombic symmetry with Pnna (52) space group where Y ion occupies 4d, 8e and 4c sites. Eu<sup>3+</sup> can thus be exchanged in YF<sub>8</sub>, YF<sub>11</sub>, and YF<sub>14</sub> coordination polyhedra. Excitation and emission spectra revealed efficient absorption into <sup>5</sup>L<sub>6</sub> energy level of Eu<sup>3+</sup> using λ<sub>exc</sub>=393 nm, producing emissions from <sup>5</sup>D<sub>1</sub> and <sup>5</sup>D<sub>0</sub> to <sup>7</sup>F<sub>J</sub> (J=0–4) energy levels. Intense red emission of Eu<sup>3+</sup> is observed, with dominant emission corresponding to <sup>5</sup>D<sub>0</sub> to <sup>7</sup>F<sub>2</sub> transition at around 611 nm.

## SILVER-BISMUTH IODIDE NANOPATELETS: SYNTHESIS, CHARACTERIZATION AND ELECTRONIC STRUCTURE

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2D layered halide perovskites gained significant research interest since they exhibited promising luminescent properties favorable for photovoltaics, photodetectors, etc. Recent studies revealed that the electronic structure of layered perovskites may depend on particle size i.e., the number of layers. This is the consequence of the quantum size effect, which is present in lead halide 2D perovskites [1]. Conversely, some lead-free 2D perovskites don't manifest a quantum size effect with size reduction. In our previous study, we successfully synthesized lead-free silver bismuth iodide (Ag-Bi-I) rudorffite nanospheres and studied their electronic structure by using X-ray aerosol photoelectron spectroscopy (XASP) [2]. In this study, we presented the fabrication of Ag-Bi-I rudorffite nanoplatelets for the first time. We investigated their structure using x-ray diffraction crystallography (XRD) and morphology by using atomic force microscopy with particle size analysis (AFM). We studied the electronic structure of obtained nanoparticles by combining XASP and conventional X-ray photoemission spectroscopy (XPS) and their optical properties by using UV-Vis absorption spectroscopy and photoluminescence spectroscopy (PL). Obtained results are compared with the DFT calculations for the examination of the quantum size effect possibly presented in our 2D layered nanosystem [3].

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## TAILORING OF Cr<sup>3+</sup> EMISSION BY TUNNING CRYSTAL FIELD IN LiAl<sub>5-x-y</sub>Mg<sub>x</sub>Si<sub>y</sub>O<sub>8</sub>

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Materials doped with Cr<sup>3+</sup> ions exhibit important properties that are used in a variety of applications, including lasers, fiber-optic thermometers, in vivo imaging, and others. The Cr<sup>3+</sup> ion's 3d<sup>3</sup> electron configuration produces deep-red emission from optical transitions between d-d orbitals, making it suitable for phosphor applications. Two overlapping emissions from the Cr<sup>3+</sup> spin-forbidden <sup>2</sup>E<sub>g</sub> → <sup>4</sup>A<sub>2g</sub> and the spin-allowed <sup>4</sup>T<sub>2g</sub> → <sup>4</sup>A<sub>2g</sub> electronic transitions are strongly dependent on the strength of the crystal field. In this work, we hypothesize that the position of the <sup>4</sup>T<sub>2g</sub> parabola can be modulated by the host material's crystal field strength through the modification of the metal-to-oxygen ionic distances. In that perspective, it is expected that tailoring of emissions will be possible by adding impurities to the host and consequently, the immediate vicinity surrounding the Cr<sup>3+</sup>.

LiAl<sub>4.95</sub>Cr<sub>0.05</sub>O<sub>8</sub> phosphor was chemically modified by the replacement of Al<sup>3+</sup> with Mg<sup>2+</sup> and Si<sup>4+</sup> ions resulting in the LiAl<sub>4.95-x-y</sub>Mg<sub>x</sub>Si<sub>y</sub>Cr<sub>0.05</sub>O<sub>8</sub> (x = y = 0.05; 0.1; 0.15 and 0.2) composition. The samples were obtained by simple polymer-assisted combustion synthesis and their structure was checked using X-ray diffraction measurements. Obtained diffractograms revealed that a cubic P4332 (212) space group, with Al<sup>3+</sup> in tetrahedral 8c and octahedral 12d sites, was preserved in all samples. Room temperature diffuse reflectance spectra clearly display three broad peaks placed around 276 nm, 370 nm, and 560 nm. The two broad absorption bands observed around 370 nm and 560 nm arise from the spin-allowed d-d transitions of octahedral Cr<sup>3+</sup> ions and have been assigned to <sup>4</sup>A<sub>2</sub> → <sup>4</sup>T<sub>1</sub> and <sup>4</sup>A<sub>2</sub> → <sup>4</sup>T<sub>2</sub> electronic transitions, respectively. The band in the UV region placed around 276 nm has been assigned to the charge transfer band of Cr<sup>3+</sup> – O<sup>2-</sup>. Photoluminescent emission spectra recorded at room temperature revealed that the increased Mg<sup>2+</sup> and Si<sup>4+</sup> content in the structure lead to the broadening of the Cr<sup>3+</sup> emission indicating the change in the coordination environment around Cr<sup>3+</sup>. Further research at low temperatures, where the vibronic influence will be reduced, will provide a more detailed analysis of the system.

## Materials for hydrogen storage

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The matter of thermodynamic barriers in the decomposition of magnesium hydride is the subject of many scientific studies, primarily through the process of destabilization of the hydride structure [1]. The most commonly used method for hydride destabilization is nanostructuring by mechanical milling which leads to a reduction in the particle and crystallite size of the  $\text{MgH}_2$  powder. Nanostructuring is often combined with catalyst addition and composite formation [2,3]. The most of research is focused on the morphological, structural, and thermodynamic effects typical for long milling times. The kinetics and thermodynamics of hydrogen uptake/release remain the main drawback for the practical application of magnesium hydride ( $\text{MgH}_2$ ) since its high thermal stability. The particle size is reduced and the specific surface area of the material is increased, which shortens the desorption path of hydrogen, thereby accelerating the desorption process and reducing the desorption temperature. Ion bombardment introduces vacancies, dislocations, and microchanges into the material surface layer, increasing the number of nucleation centers. While mechanical milling represents the simple and fast way for structure destabilization, thin films are a great way to monitor the influence of microstructure and/or additives on sorption properties under controlled conditions. They are particularly suitable because ion bombardment can be used to control a certain concentration of defects at certain depths by simulation predictions. During mechanical milling, various additives are added to act as so-called catalysts and/or milling agents, which may produce additional defects, delay agglomeration, and thus improve the sorption properties of  $\text{MgH}_2$ . This study aims to investigate the effect of defects in the volume and on the surface of the material. The first part will deal with the influence of defects created in volume, on composites synthesized by mechanical milling at different parameters and different amounts of additives. The second part deals with the study of the influence of surface defects on sorption properties by bombarding thin films with  $\text{H}^-$  and  $\text{Xe}^{8+}$  ions.



## **VLATACOM INSITUTE CURRENT AND FUTURE PROGRAM – CHALLENGES FOR SPECIAL MATERIALS AND TECHNOLOGIES**

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This presentation gives introduction about Vlatacom Institute development from 1997, when the company was founded, until today when the company acts as research and development Institute with primary focus on the international market. The program covers applied cryptography, electro-optical systems, high frequency over-the-horizon radar, command and control systems, ICT solutions for government applications, smart ammunition, guidance systems, anti-drone solutions and civilian application of mentioned activities in smart cities projects. Besides these ongoing projects we will also give roadmap for future activities like laser weapons, satellite program and sea-drone platform. In this presentation special attention is given to the needs for special materials and technologies for their application

**VLATACOM SOLUTIONS IN AREAS OF APPLIED CRYPTOGRAPHY,  
RADAR SYSTEMS, ELECTRO-OPTICAL SYSTEMS, ADVANCED  
WEAPONS AND ICT TECHNOLOGIES**

*Vlatacom Institute, Bulevar Milutina Milankovića 5, 11070 Belgrade, Serbia,*

Vlatacom Institute has world-class solutions in areas of cryptography, high frequency over the horizon radars (HF-OTHR), electro-optical systems, advanced weapons, software solutions and ICT systems. In applied cryptography area the focus is on unique solutions for voice encryption, cryptographic key agreement based on EEG signals and steganography for hiding encryption context from massive interception systems. HF-OTHR solutions utilizes cutting-edge technology of hardware design and signal processing that enables successful and very cost-effective protection of marine exclusive economic zones. Electro-optical systems designed by Vlatacom institute are fusion of the latest sensors in various spectral ranges together with signal processing platforms that efficiently run artificial intelligence based algorithms for target detection and tracking. Advanced weapons are a clear example of multi-disciplinary projects that require fusion of mechanical design, special materials, sensors, ruggedized electronic components and signal processing. The specialty of Vlatacom Institute's ICT solutions is its country level application which require special approach in system architecture, implementation, testing and maintenance.

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