

The 2nd Serbian Conference on Materials Application and Technology - SCOM

BOOK OF ABSTRACTS

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SCOM 2023

**The 2nd Serbian Conference on Materials
Application and Technology**

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Belgrade, Serbia, 18th - 20st of October 2023

Dear Colleagues and Friends,

It is our great pleasure to welcome you to the second Serbian Conference on Materials Application and Technology - SCOM2023. 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, SCOM2023 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, five tutorial lectures, five 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 SCOM2023 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 SCOM2023 wish you a nice time during the conference in Belgrade!

Conference Chairperson

Prof. Dr. Miroslav D. Dramićanin

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HIGH-PRESSURES IN PHYSICAL SCIENCES

Andrzej Suchocki

Institute of Physics, Polish Academy of Sciences, 02-668 Warsaw, Poland

Pressure is one of the fundamental thermodynamic variables, which allows for precise changing (decreasing) the interatomic distances and altering the bonding patterns of materials, leading to phase transformations into high-pressure structures with different and often unusual chemical and physical properties. These structures are sometimes metastable, which means that after the pressure-induced phase transformation, they remain stable at ambient pressure. The best-known example of high-pressure induced phase transformation is the change of graphite (a soft material with an sp^2 C–C bonding) into a diamond (the hardest known material with an sp^3 C–C bonding), which is stable at ambient pressure [1].

High pressures are also very important for superconductor research, as only 30 elements exhibit superconductor properties under normal conditions. Application of high pressures transforms 25 others into a superconducting phase [2]. High pressures are also indispensably important for studying new high-temperature superconductors.

High pressures can effectively lower the barrier of the chemical reactions and thus make the chemical reaction possible only at HP conditions. HP synthesis of functional exotic materials with desirable chemical or physical properties via a chemical reaction of distinct species is a very important method of their production, used for the preparation of hydrogen storage and superhard novel materials. High pressures, met in the Earth's core interior, and in the other planets and stars, can be used for controlled permutation of matter into functional materials for more efficient solar cells [3].

High pressures are very important in geology. Researchers examine many materials to reveal the processes occurring in Earth's mantle and crust, which should allow for predicting earthquakes. New forms of minerals are synthesized during these studies, such as recently prepared synthetic ringwoodite, a high-pressure polymorph of olivine (magnesium iron silicate) which is the rarest mineral on the Earth [4].

The pressures achieved in the special construction of diamond anvil cells now reach about 500 - 600 GPa (there is some information on reaching even higher pressures). At this pressure, it was expected that hydrogen would become metallic. Recently it has been reported achieving this "holy grail" of high-pressure research [5]. Higher pressures up to about 5 TPa can be recently achieved in the National Ignition Facility with the use of 2MJ lasers designed to create thermonuclear fusion in the laboratory [6].

High pressures are also a very important research tool, especially for studying the properties of new phosphors. High pressures allow for precise tuning of their properties such as band-gap, positions of certain electronic levels of the dopants relative to the band structure and also to the vacuum level [7] spectral properties of certain electronic transitions, the energy of phonons, conductivity, magnetic properties, crystallographic structure, and other related features [8],[9].

Knowledge of the pressure at which such an effect occurs leads to the replacement of externally applied pressure by the "chemical pressure", i.e. changes of the lattice parameter of the crystal by proper substitution by the cations with smaller ionic radii and obtaining this way

efficient phosphor at ambient pressure. Such effect allows using so-called “band-gap engineering”, which also provides a possibility of independent control of the certain deep trap levels responsible for luminescence quenching, which could have detrimental effects on the scintillating properties of certain materials.

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**POINT DEFECTS IN BINARY OXIDES AND HALIDES: OPTICAL
PROPERTIES AND SOME APPLICATIONS**

Anatoli Popov

Institute of Solid State Physics, University of Latvia, Riga, Latvia, popov@latnet.lv

The abstract will be provided by the author.

CONTROL OF DEFECTS IN OPTICAL MATERIALS AND FOCUS ON APPLICATIONS OF PERSISTENT PHOSPHORS

Bruno Viana

IRCP; Chimie-ParisTech, PSL University, 11 rue Pierre et Marie Curie, 75005 Paris, France

The development of luminescent materials requires materials with high fluorescence intensity but also with careful control of the defects which could affect the kinetic and intensity of the luminescence. In some applications, as Scintillation, defects/traps must be carefully controlled to avoid room temperature detrapping and afterglow emission. Additionally in bioimaging there is a recent large interest for materials with long persistent luminescence. Several new applications are envisioned with these materials including theranostic and sensing properties: At nanoscale, deep red and near-infrared persistent luminescence nanoparticles enable highly sensitive in vivo optical detection and complete avoidance of tissue autofluorescence. Persistent luminescence can be activated in vivo through living tissues using highly penetrating low energy photons. Surface functionalization of this photonic probe can be adjusted as well as the wavelength of the optical stimulation to favor multiple challenging biomedical applications. At larger size persistent large crystals recently can be interesting in jewelry and lighting applications. Examples will be presented during the seminar.

Brief introduction

Dr Bruno Viana is a CNRS Senior Scientist at the Chimie-Paristech Institute and Professor at PSL University, Paris, France. He works on materials synthesis at different sizes from nanometric to centimetric sizes and their characterization for photonics applications including lasers, scintillation, imaging and lighting. He has recent focus on materials for bio-imaging with persistent luminescence and for nanothermometry. Dr Viana is the author of 25 patents and about 360 publications and several book chapters, h factor of 71 and about 18,000 citations (Google Scholar).

FUNDAMENTALS OF OPTICAL OXYGEN SENSING

Sergey Borisov

Graz University of Technology, Institute of Analytical Chemistry and Food Chemistry,
sergey.borisov@tugraz.at

This tutorial talk will focus on basics of optical oxygen sensing, which have become a technique of choice in numerous scientific and industrial applications. After introduction into luminescence-based chemical sensors, the talk will cover luminescence quenching by molecular oxygen, important classes of indicator dyes, composition of oxygen sensing materials, formats of oxygen sensors including planar optodes, fiber-optic sensors and nanoparticles, and finally highlight a few important applications.

TEMPERATURE IMAGING USING INORGANIC PHOSPHORS: METHODS AND APPLICATIONS

Benoit Fond

Department of Aerodynamics (DAAA), ONERA, the French Aerospace Lab, Paris Saclay

Using the temperature dependent luminescence of inorganic phosphor particles, it is possible to remotely measure the internal temperature distribution within a transparent fluid or solid by introducing the particles in the medium or to measure the temperature distribution of a surface over which particles are deposited.

Such minimally intrusive measurements permit to probe with a very fine spatial and temporal resolution the thermal dynamics of systems of interest, for example a chemical reactor, a fluid mechanical experiment of geophysical relevance or an aerodynamical model in a wind tunnel.

The temperature can be derived from the temporal dynamics of the luminescence emission or from its spectral content. Both response are self referenced, i.e, they measure relative changes in luminescence intensity which are robust against variations in illumination power or particle concentrations.

In this talk, we will review the various measurements configurations for this concept and focus on a few example applications, to work through the experimental need, the choice of measurement strategy including luminescent material, and finally the utilisation of the measurements.

LUMINESCENT THERMOMETRY METHODS BASED ON THE NEAR- INFRARED EMISSION OF Mn⁵⁺-ACTIVATED Ca₆Ba(PO₄)₄O PHOSPHOR

*Željka Antić, Sanja Kuzman, Zoran Ristić, Ivana Zeković, Miroslav D. Dramićanin
Center of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences, National
Institute of the Republic of Serbia, University of Belgrade, 11001 Belgrade, Serbia,
zeljkaa@gmail.com*

For the purpose of near-infrared luminescent thermometry, we present a demonstration of the capabilities of the Mn⁵⁺-doped Ca₆Ba(PO₄)₄O phosphor. The CaCO₃, BaCO₃, (NH₄)H₂PO₄ and MnO that made up the substance's precursors were used in the traditional solid-state process that was used to synthesis the material. The steady-state method enabled quick measurements of emission spectra, which led to the collection of a large number of spectra for each temperature point. These spectra were subsequently put to use in the process of determining the experimental temperature resolution for each thermometric method. Conventional luminescence thermometry was utilized in order to measure and analyze temperature-dependent near-infrared emission features. These features included intensities of emission band, as well as emission band energies and bandwidths. After that, these data are utilized in the performance of three distinct types of thermometry that are based on a single parameter, as well as multiparametric thermometry that is based on multiparametric linear regression.

RARE EARTH DOPED NIOBATES FOR UC LUMINESCENCE APPLICATIONS

Tamara B. Ivetić^a, Boris Banjac^a, Ljubica Đačanin Far^b, Zoran Ristić^b

^a*University of Novi Sad Faculty of Sciences, Department of Physics, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia, tamara.ivetic@df.uns.ac.rs*

^b*Center of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, 11001 Belgrade, Serbia*

Oxide compounds of the niobate type with the composition ANbO_4 ($A = \text{Lu, Y, La, Gd}$) have promising properties as inorganic luminescence host materials [1-5]. The luminescence process of converting lower-energy, long-wavelength NIR light into higher-energy UV or VIS light, known as the luminescence up-conversion (UC) phenomenon, finds wide application in optical and sensor devices and bio-medical imaging and therapy [6]. The UC of rare-earth (RE)-based materials appears mainly through excited-state absorption, energy-transfer upconversion, and photon avalanche mechanisms, the latter of which is rarely found. Niobates ANbO_4 ($A = \text{Lu, Y, La, Gd}$) show energy-transfer UC luminescence when doped with Er^{3+} , Ho^{3+} , and Tm^{3+} ions as activators and often co-doped with Yb^{3+} ions as sensitizers [7]. The choice of yttrium niobate (YNbO_4) as the matrix and rare-earth ions of erbium/ytterbium for UC activation seems preferable because YNbO_4 has low phonon energy, is both chemically and thermally stable as a host material, with a fairly simple synthesis, while Er^{3+} as an activator has a suitable energy level spacing and can be excited by several IR wavelengths, and Yb^{3+} as a sensitizer has a higher probability of absorption under 980 nm excitation which can increase the energy-transfer UC [8]. In our recent study, erbium (1 at. %) and ytterbium (2 at. %) doped yttrium niobate ($\text{YNbO}_4:\text{Er,Yb}$) nanocrystallites of about 31 nm were synthesized using a combustion-assisted solid-state method. Scanning electron microscopy showed uniformity of shape and particle size of several microns and no RE-dopants affecting the microstructure. Energy dispersive spectroscopy mapping confirmed the satisfactory quality of doping. Emission spectra at 980 nm excitation showed a total of 4 Er^{3+} emission bands from the UC process. To determine the variation of emission characteristics with temperature, the phosphor thermometry decay measurement method was used. The quality and potential of $\text{YNbO}_4:\text{Er,Yb}$ as a temperature sensor was quite good as the relative sensitivity decreased from 0.2% to 0.09% K^{-1} by varying the temperature from 300 to 600K.

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MESOPOROUS SILICA AND ORGANOSILICA NANOPARTICLES FOR APPLICATIONS IN CANCER THERANOSTICS AND PROTECTION OF SKIN

Nikola Ž. Knežević, Mirjana Mundžić, Aleksandra Pavlović, Minja Mladenović
BioSense Institute, University of Novi Sad, Dr Zorana Djindjica 1, 21000 Novi Sad, Serbia.,
nknezevic@biosense.rs

The use of nanomaterials is ever increasing in various application areas due to stringent efforts of researchers in different scientific fields. Our research focuses on the synthesis of mesoporous silica (MSN) and organosilica nanoparticles (PMO), their functionalization and application in targeted treatment and diagnostics (theranostics) of cancer,[1] protection of skin from UV irradiation,[2] nanocomposite coatings,[3] and in construction of sensors.[4] Herein, our recent results are presented in the area of pH-responsive delivery of anticancer drug paclitaxel (PTX) to brain cancer (Glioblastoma multiforme) cells, as well as in the area of using magnetic resonance imaging (MRI) for image-based monitoring of cancer treatment. The effect of the presence of cancer-targeting peptide on the surface of nanoparticles was also evaluated in terms of its effects on toxicity of nanoparticles, as well as through the capabilities to penetrate cancer cells, by confocal microscopy and flow cytometry.

Characterization of all prepared nanomaterials is performed by SEM, TEM, TGA, XRD, DSC, zeta potential. UV/VIS, FTIR, and fluorescence spectroscopy, while their toxicity and uptake ability was evaluated on U87 cell lines *in vitro*.

Furthermore, novel results on synthesis and characterization of novel PMO-based materials for protection of skin from harmful UV irradiation are to be discussed.

Acknowledgements

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LASER-MODIFIED NANOGRAINED Ti-45Nb ALLOY'S PERFORMANCE IN BIO-ENVIRONMENT

Ivana Cvijović-Alagić^a, Slađana Laketić^a, Miloš Momčilović^a, Jelena Bajat^b, Jovan Ciganović^a,
Vesna Kojić^c, Đorđe Veljović^b

^a*Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of
Belgrade, Serbia, ivanac@vinca.rs*

^b*Faculty of Technology and Metallurgy, University of Belgrade, Serbia*

^c*Oncology Institute of Vojvodina, University of Novi Sad, Serbia*

The most commonly used metallic implant materials for hard tissue replacements in orthopedic and dental surgery nowadays are commercially pure titanium (CP-Ti) and ($\alpha+\beta$) Ti-based alloys due to their superior biomechanical compatibility in comparison to other biometallics. However, these Ti-based materials still do not meet all implantation requirements for their long-term use in physiological conditions because of their somewhat limited resistance to tribo-corrosive degradation in harsh bio-environments and/or adverse health effects initiated by the presence of cytotoxic elements in their composition. Accordingly, revision surgery is needed ten years after the prime replacement surgery limiting in that way the active life of surgical patients. Since the β -type Ti alloys, which contain non-toxic elements, can exhibit improved biocompatible properties compared with other Ti-based materials their potential application in medicine is in the last few years carefully considered.

The Ti-45Nb (mass%) alloy, as the β -type Ti alloy, shows significant potential for application in orthopedic and dental surgery. Nevertheless, its performance in the bio-environment can be additionally improved to maximize its medical applicability. Necessary improvements can be achieved by the alloy's microstructural and surface modifications using the appropriate processing procedures that can ensure the obtainment of favorable alloy biocompatible properties. Structural and surface modification methods that can be successfully used for the attainment of more durable hard-tissue implants are, above all others, high-pressure torsion (HPT) and laser surface scanning, since the HPT processing leads to the grain refinement and the obtainment of ultra-fine grained (UFG) microstructure with higher compatibility with biological systems, while the laser surface scanning influences the formation of protective surface scales and the appearance of developed bio-active surface.

The research scope was therefore to explore the achievement of improved corrosive and biocompatible response of the Ti-45Nb alloy in simulated physiological conditions through the alloy additional processing with combined HPT and laser irradiation procedure. The alloy's microstructural, electrochemical, and cytotoxic characteristics were evaluated before and after its additional processing. Research results showed that the 14 times smaller grains, obtained through the HPT processing, and the appearance of laser-induced morphologically altered and highly oxidized surface led to the significant improvement of the alloy corrosion resistance and the cells-implant interaction. Moreover, the intensification of laser beam and alloy interaction in air by an increase of the laser output energy from 5 mJ to 15 mJ led to a more intensive formation of the protective surface oxide scales and at the same time boosted the viability of cells in contact with the Ti-45Nb alloy from excellent 127.18% to superior 134.42%. The controlled alloy microstructural and surface alterations also resulted in the appearance of a compact and protective bi-modal external oxide scale in the simulated body conditions that simultaneously enhanced the alloy's resistance to corrosion degradation, and cell proliferation and growth. Accordingly, the combined HPT and laser irradiation treatment can be considered an excellent alloy processing method for the successful improvement of biometallic's performance in a bio-environment.

FABRICATION OF HIGHLY-TRANSPARENT CERAMICS FROM TRULY NANO-SCALED PARTICLES

Maxim Ivanov

Center of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, PO Box 522, 11001 Belgrade, Serbia

E-mail: maxim887@yahoo.com

Development of new technologies to produce highly transparent ceramics needs application of ever smaller particles of starting materials. Optimized methods, like homogeneous precipitation or combustion technique, can produce inorganic submicronic particles with a narrow size distribution. However, to accomplish high-quality, truly nano-scaled particles, new methods of preparation are still of high interest. Among a number of fabrication methods for true nanoparticles, laser synthesis (laser supported material evaporation and subsequent vapor condensation) and self-propagating high-temperature synthesis (SHS) are quite promising, since they yield pure, weakly agglomerated, spherical nanoparticles with a narrow size distribution [1,2]. Such nanoparticles could lead to an excellent optical material, if one can learn how to transform them to nanocrystalline, fully dense ceramics. Among green-body forming techniques, colloidal methods of tape, slip castings and electrophoretic deposition are particularly prominent to fabricate thin films and ceramics. The methods need an organic dispersant to stabilize suspensions of particles, but the dispersants are mostly developed to stabilize micron and submicron particles and not predictable efficient, especially taking in account complicated surface chemistry, in the case of nanoparticles.

The presentation deals with the nanoparticles fabrication technologies and techniques of compacting the nanoparticles into flaw-free green body to sinter highly transparent ceramics.

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MODIFICATION OF TiO₂ NANOPARTICLES WITH DIHYDROQUERCETIN: CHARACTERIZATION, CYTOTOXICITY AND ANTIMICROBIAL ABILITY

Valentina Z. Nikšić¹, Miljana M. Dukić¹, Andrea M. Pirković², Vesna M. Lazić¹, Jovan M. Nedeljković¹

¹*Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia*

²*INEP Institute for Application of Nuclear Energy, University of Belgrade, Belgrade, Serbia*

The aim of this study is to modify the surface of TiO₂ nanoparticles with the bioactive ligand dihydroquercetin (DHQ) to form an interfacial charge transfer complex (ICT). The ICT complex, TiO₂/DHQ, will be active under visible light. DHQ is a catechol-type ligand with pronounced antioxidant and valuable biological performance.

The inorganic-organic hybrid nanocomposite TiO₂/DHQ was characterized by Fourier-transform infrared (FTIR) and Reflectance spectroscopy. FTIR spectra identified C=O stretching of flavonoids, O-H, C-O, and C-O-C stretching of phenolic compounds, confirming the presence of ligands on the surface of TiO₂ nanoparticles. The Kubelka-Munk transformation of the diffuse reflection spectra shows a shift in the excitation of the TiO₂/DHQ towards the visible part of the spectrum. The binding of DHQ to the TiO₂ NPs surface induced a change in the color of the solid material from white (TiO₂) to light-brown (TiO₂/DHQ).

Cytotoxicity testing was performed on healthy human MRC-5 cells and human cervical cancer HeLa cells determined by MTT assay. Additionally, the effect of TiO₂/DHQ on the production of reactive oxygen species in MRC-5 and HeLa cells was investigated using the H2DCFDA assay. Finally, the antimicrobial properties of the TiO₂/DHQ nanocomposite material under visible light (437 nm) were tested against the bacteria *E. coli* and *S. aureus*.

VISIBLE-LIGHT-RESPONSIVE ZnO-BASED ICT COMPLEXES WITH CATECHOLATE- AND SALICYLATE-TYPE LIGANDS: SYNTHESIS, CHARACTERIZATION, AND APPLICATION IN ENHANCED HYDROGEN PRODUCTION

Miljana Dukić, Valentina Nikšić, Dušan Sredojević, Vesna Lazić, Jovan M. Nedeljković
Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia

This study presents a significant advancement in the development of materials capable of harnessing solar energy for various applications, including energy conversion. The synthesis, characterization, and application of visible-light-responsive ZnO-based Interfacial Charge Transfer (ICT) complexes functionalized with catechol- and salicylate-type ligands were investigated. Through meticulous chemical processes, ZnO nanoparticles were combined with colorless benzene derivatives containing catechol and salicylate ligands, marking the first successful formation of complexes with unique light-absorbing capabilities. To gain insights into the optical properties and surface structures of these complexes, a multifaceted analytical approach was employed. Reflection and infrared spectroscopic techniques were utilized to probe the electronic transitions and vibrational modes within the complexes. The experimental observations were bolstered by density functional theory (DFT) calculations, providing a comprehensive understanding of the energy levels and binding configurations at play in these hybrid systems. The condensation process between the hydroxyl groups on the surface of ZnO and the organic components occurred as ligand molecules formed strong chemical bonds with the zinc atoms. The practical implications of these ICT complexes were evaluated in the context of light-driven reactions, particularly in water-splitting reactions for hydrogen production—a critical component of sustainable energy technologies.

The results were promising, as ZnO nanopowders modified with catechol or caffeic acid demonstrated hydrogen production rates exceeding 50% higher than their unmodified counterparts. Importantly, these materials exhibited consistent hydrogen production over extended periods, highlighting their stability and reliability. In conclusion, the synthesis of visible-light-responsive ZnO-based ICT complexes with catechol- and salicylate-type ligands contributes to the growing body of knowledge in the field of materials science, offering innovative solutions for a greener and more energy-efficient future.

GRAPHENE-BASED MATERIALS AND THEIR HYDROGEN BINDING PERFORMANCE. A DFT STUDY

Michal Malček

Institute of Physical Chemistry and Chemical Physics, Faculty of Chemical and Food Technology, Slovak University of Technology, Bratislava, Slovakia, michal.malcek@stuba.sk

Since the re-discovery of graphene in 2004 [1], the graphene-based nanomaterials have attracted a considerable interest due to their unique properties. Modification of the graphene surfaces with heteroatoms may significantly improve their electronic properties and chemical reactivity. In the presented work, three types of graphene-like surfaces modified with first row transition metals (TMs) are investigated at the DFT level of theory: i) circumcoronene, a polyaromatic hydrocarbon composed of 54 carbon atoms arranged in 19 hexagonal rings, is used as a model system of the finite graphene quantum dot [2, 3]; ii) rectangular graphene surface unit composed of 48 carbon atoms is used as a supercell in periodic calculations, representing an infinite model [4]; iii) a fullerene subunit circumtrindene, C_{36} , is a bowl-shaped polyaromatic hydrocarbon composed of five- and six-membered rings [5]. A scheme of all these structures doped with TM atom is illustrated in Figure 1.

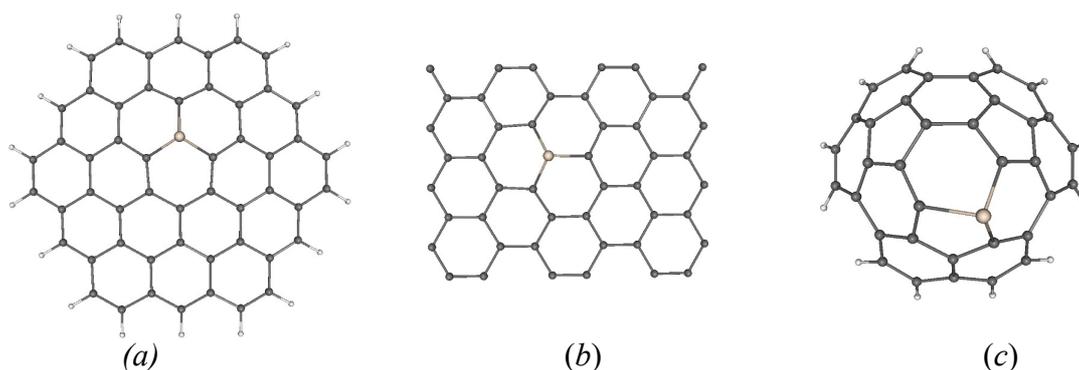


Figure 1: TM-doped circumcoronene (a), TM-doped graphene surface (b), TM-doped C_{36} (c).

The TM atom within the studied structures represents an active site for the attack of H_2 molecule. Using the DFT calculations as well as the QTAIM and PDOS analysis we have confirmed that the adsorption limit is three H_2 molecules symmetrically arranged in the vicinity of one TM atom [4,6,7].

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ELECTRON PARAMAGNETIC RESONANCE IN THE INVESTIGATION OF MATERIALS' ACTIVITY: FROM TRANSITION METALS COMPLEXES TO PHOTOCATALYSIS

Miriam Malček Šimunková^a, Zuzana Barbieriková,^a Dana Dvoranová,^a Vlasta Brezová,^a
Marián Valko,^a

^a Institute of Physical Chemistry and Chemical Physics, Slovak University of Technology,
Bratislava, Slovakia, miriama.simunkova@stuba.sk

EPR spectroscopy depends on the absorption of electromagnetic radiation like any other spectroscopic technique. Its uniqueness is the ability to measure paramagnetic samples in a very sensitive and non-destructive manner [1]. The detection of radical species is an important part in the evaluation of studied material activity.

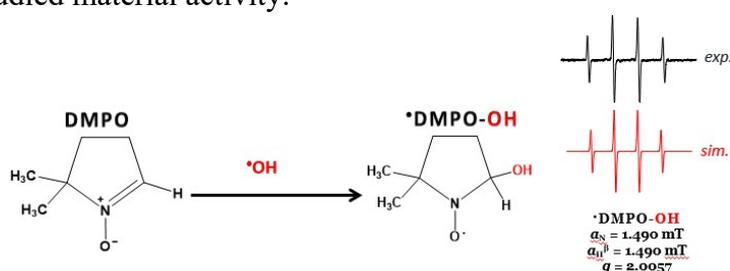


Fig.1 DMPO as a spin trap for trapping hydroxyl radical

Another possible application in the study of transition metal coordination compounds is the change of spectral parameters reflecting the differences in local environment and geometry of prepared complexes. A very important aspect of using EPR in the investigation of their activity is the model Fenton system [2] with the addition of spin trap DMPO (5,5-dimethyl-1-pyrroline N-oxide). This method is based on the chemical reaction of a diamagnetic spin trap (ST) with a short-lived radical, producing a more stable nitroxide radical, *i.e.*, spin-adduct, using nitrones, *N*-oxides and nitroso compounds as the spin trapping agents (Figure 1). In all cases, we propose that the interaction of a superoxide radical anion with the redox metal ion moiety in the complexes gives rise to redox cycling reactions with concomitant production of free radicals *via* the Fenton reaction – e.g. $\cdot\text{OH}$. Anti vs. pro-oxidant behaviour of such complexes can be evaluated based on the qualitative (identification of radical species) and quantitative (amount of free radicals trapped in the model system) analysis. EPR spectroscopy occupies an exclusive position in the investigation of titania dioxide based photocatalysts [3], providing a characterization of paramagnetic centres produced via the trapped photogenerated electrons and holes and materials with transition-metal ions doping. Much of the research exploiting EPR spectroscopy deals with the investigation of reactive radical intermediates produced in the irradiated TiO_2 particulate systems where the application of an indirect spin trapping technique is inevitable. In the literature hydroxyl radicals are frequently declared as the most important reactive species generated upon TiO_2 irradiation.

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MODIFIED TiO₂ WITH SALICYLIC ACID DERIVATIVES AS ICT COMPLEXES

Zuzana Dyrčiková, Miriama Malček-Šimunková, Karol Lušpai, Dana Dvoranová
*Institute of Physical Chemistry and Chemical Physics, Faculty of Chemical and Food
Technology, Slovak University of Technology in Bratislava, Radlinského 9, Bratislava, SK- 812
37, Slovak Republic, zuzana.dyrcikova@stuba.sk*

As the world's population grows, so do its demands on living standards. Industrial progress also brings new challenges, such removal of diverse pollutants. In this case, conventional methods are no longer sufficient, and attention of the scientific community is turning to newer processes that would be more efficient, environmentally friendly, as well as economically acceptable. The question of acquisition and storage is becoming more and more actual and interest in this field has been increasing year by year [1-2].

Nanomaterial semiconductors as titanium dioxide and zinc oxide are extensively studied due to their wide applications. They are mainly used for water splitting, removal of organic and/or inorganic pollutants, in solar cells and their potential extends to other possible applications. Interest about these oxides is mainly involved by high chemical stability, low cost, and photocatalytic activity. For the field of heterogeneous photocatalysis is their limitation in absorption radiation only in UV region, which represent only 5% of solar energy. This involved wide band gap for TiO₂ (anatase) ~3,2 eV and ZnO ~3,3 eV. To shift their photocatalytic activity to the visible-light region, different ways of their modification are applied. One approach to extend absorption of TiO₂ into a more practical range of the solar spectrum is emerging is to utilize an interfacial charge transfer (ICT) surface modifier into the conduction band of semiconductor particles. In recent years, the counterpart components of the metal-oxide based ICT complexes have been small, colourless organic molecules such as phenol, catechol, or small non-aromatic molecules formed as interfacial charge transfer (ICT) complexes between wide band gap metal oxides [1-4].

Our research focuses on creating and characterising titania surfaces treated using salicylic acid derivatives. The ICT complexes were prepared *via* environmental-friendly technique in aqueous suspensions utilising the condensation reaction of the hydroxyl groups from the inorganic and organic components of the hybrid. Spectroscopic methods as Raman, IR, UV/Vis are utilized to characterize the prepared materials. Applying of indirect electron paramagnetic resonance (EPR) spectroscopy techniques, *e. g.*, spin trapping, spin scavenging or photoinduced reduction, the photocatalytic activity is monitored. In the ongoing study we anticipated that exposure to visible light will lead to the greater photocatalytic activity of ICT complexes.

Keywords: Interfacial Charge Transfer, Titanium Dioxide, Zinc Oxide, Surface-modification.

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ECO-FRIENDLY, FLUORESCENT, FUNCTIONALIZED GRAPHENE QUANTUM DOTS: COMPARATIVE SYNTHETIC STUDY AND FUTURE PROSPECTS

Dorđe Trpkov^a, Dragana Tošić^a, Jelena Pajović^b, Dušan Sredojević^a, Milica Vinić^c, Radovan Dojčilović^a, Miloš Ognjanović^a, Dušan K. Božanić^a, Vladimir Đoković^a

^a*Institute of nuclear sciences "Vinča", University of Belgrade, Belgrade, Serbia*
djordjet@vinca.rs

^b*Faculty of Physics, University of Belgrade, Belgrade, Serbia*

^c*Institute of Physics-Belgrade, University of Belgrade, Belgrade, Serbia*

Graphene quantum dots (GQD) were prepared by both "bottom up" hydrothermal methods and "top-down" laser ablation of graphene target. The synthetic routes were determined according to their simplicity and sustainability. Throughout the procedures abundant, low-cost and eco-friendly chemicals were used, such as citric acid, urea, glycine and amino acids. Complicated purification steps were avoided, while keeping sample quality and the distribution of particle sizes within the nanometer range. In addition, to tune the optical properties of GQD, the particles were non-covalently functionalized by L-Phenylalanine (L- Phe) and L-Tryptophan (L-Trp) biomolecules. An overview of methods used for the fabrication of either pristine or functionalized graphene quantum dots is presented. Fluorescence of GQD systems, which arises from its chemical functionalities, covered the spectral range from blue to yellow. In parallel to the experimental investigation, we used density functional theory (DFT) to quantify stacking and hydrogen-bonding interactions between nitrogen doped GQDs and amino acids, based on the assumed GQD chemical structure. This study offers evaluation and optimization of known GQD synthetic routes in order to fit future application prospects, such as bioimaging and drug delivery.

TRACKING PROTEIN NETWORK DYNAMICS: THE CASE OF THE EXOCYTOSIS

Radovan Dojčilović^{a,b}, Sebastian Ortiz^b, Marta Puig^b, Sasha Meek^b, Oriol Gallego^b

^a*Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia.*

^b*Department of Medicine and Life Sciences, Universitat Pompeu Fabra, Barcelona 08005, Catalonia, Spain.*

Within the general landscape of vesicle trafficking, the constitutive exocytosis represents a process by which vesicles are transported and fused with the cell membrane. This is done to release molecules and supply the membrane with lipids and proteins. Budding yeast is an attractive model organism to study exocytosis due to the large collection of characterized mutants and well-established conservation of function in mammalian cells. In the process of exocytosis, a complex dynamic network of proteins is involved, and the mechanisms of action of proteins involved in transport, tethering, fusion, and recycling still remains unclear. By using fluorescence microscopy and tracking methods for proteins in live cell imaging, we are able to start constructing the exocytosis timeline, and to quantitatively investigate stoichiometry of exocytic sites. In the present study, we will focus on the methods for analyzing protein dynamics in the case of exocytosis. Studying the functional implications of these dynamic interactions and the coordination of action is crucial to our understanding of the molecular mechanism of exocytosis.

NOVEL $Y_3NbO_7:xDy^{3+}$ PHOSPHOR AND ITS TUNABLE EMISSION

Ljubica Đačanin Far, Aleksandar Ćirić, Jovana Periša, Vesna Đorđević, Zoran Ristić, Bojana Milićević, Miroslav D. Dramićanin

Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences-National Institute of the Republic of Serbia, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia,

ljubica.far@vin.bg.ac.rs

As yttrium niobates, the $Y_2O_3-Nb_2O_5$ combination exists in two forms: $YNbO_4$ and Y_3NbO_7 , and the latter has been studied as a host for photoluminescent ions to a limited extent [1-3]. In this research, the powders of $Y_3NbO_7:xDy^{3+}$ ($x = 0.5, 1, 1.5, 3$ and 5 mol%) were produced through a solid-state process. X-ray diffraction investigations confirmed the fluorite-type structure (space group $Fm\bar{3}m$) of powders with crystallite size in the range of 19–60 nm. Both the photoluminescence excitation and emission spectra revealed the presence of defects within the material. With different excitation wavelengths, the emission spectra exhibited distinct emission patterns. At each excitation wavelength, the emission was quenched at Dy^{3+} concentration higher than 1mol%. The decay time measurements of the highest intensity emission revealed a progressive decrease from 0.472 milliseconds for $x = 0.5$ mol% to 0.246 milliseconds for $x = 5$ mol%. The CIE chromaticity coordinates investigation revealed that the emission color may be altered by varying the excitation wavelength, ranging from blue (excitation at 333 nm) and near-white (excitation at 353 nm and 390 nm) to orange (excitation at 457 nm). The chromaticity of emission under 353 nm and 390 nm excitation validated the material's suitability as an almost-white phosphor.

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FROM LUMINESCENT POLYCRYSTALLINE TARGETS TO EPITAXIAL THIN FILMS BY RHEED CONTROLLED PULSE LASER DEPOSITION

Zoran Ristić^a, Aleksandar Ćirić^a, Vesna Đorđević^a, Milica Sekulić^a, Miroslav Dramićanin^a, Milan Radović^{a,b}

^a*Center of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia*
risticz@vin.bg.ac.rs

^b*Swiss Light Source, Paul Scherrer Institut, Villigen, CH-5232, Switzerland*

Luminescent transition metal-ion doped materials are of great interest in different areas - from the flat-panel displays, solid-state lighting and sensors to solar cells and collectors and many others. One of the possible ways to tailor and control the important optical parameters of such materials is to prepare them in the form of epitaxial luminescent thin films. Epitaxial films are thin layers of crystalline material grown on a substrate in such a way that their crystal lattice structure aligns with that of the substrate. Their growth relies on advanced deposition techniques such as molecular beam epitaxy (MBE), metal-organic chemical vapor deposition (MOCVD) and pulsed laser deposition (PLD). These methods allow for the precise control of crystal structure and orientation, resulting in films with high crystallinity and minimal defects. Furthermore, epitaxial growth permits deliberate dopant incorporation and modulation of composition, enabling tailored luminescent properties.

In this work a novel approach for the synthesis of luminescent thin films using the pulse laser deposition (PLD) technique, facilitated by real-time reflection high-energy electron diffraction (RHEED) for precise control of film growth and crystallinity is presented. A polycrystalline material with luminescent properties (LaAlO₃:Cr) is used as the target material and was transferred by PLD to different substrates (LaAlO₃ and SrTiO₃) forming an epitaxial thin film in the process. As a result, a functional, optically active films of different thicknesses were attained that display distinctive properties based on the substrate used.

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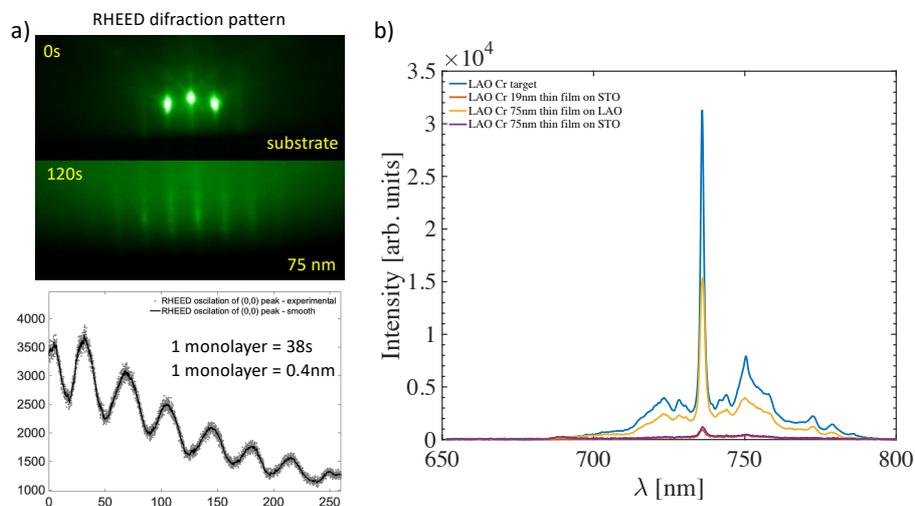


Figure 1. a) RHEED pattern and oscillation obtained during thin film growth. b) Luminescent spectra of different luminescent thin films

HIGH-RESOLUTION PHOTOLUMINESCENCE OF Pr³⁺ OR Er³⁺ DOPED OXIDES AND CORRELATIONS WITH STRUCTURAL PROPERTIES

Andrei V. Racu^{a,b}, Zoran Ristić^c, M. Ivanovici^a, R. Banică^a, Aleksandar Ćirić^c, Željka Antić^c,
Miroslav D. Dramićanin^c, Michail G. Brik^c

^aNational Institute of Research and Development for Electrochemistry and Condensed Matter, INCEMC, 144 Str. Prof. Dr. A. P. Podeanu, Timișoara, România.

^bICAM, West University of Timisoara, 4 Bd V. Pârvan, Timișoara, România.

^cCentre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia.

The utilization of photoluminescence from lanthanide dopants has been identified as a valuable technique for verifying the structural properties in different host materials [1, 2]. The Praseodymium (Pr³⁺) and Erbium (Er³⁺) ions are employed as dopants in various oxides. Through the process of upconversion photoluminescence, these ions facilitate the conversion of electromagnetic radiation from the visible (VIS) range to ultraviolet C (UVC) or from near-infrared (NIR) to visible (VIS), respectively. Light-conversion materials have diverse uses ranging from anti-counterfeiting labels to biological markers, as well as UVC bactericidal coatings. However, in certain instances, such as in the case of Y₂SiO₅:Pr³⁺, there is a need to enhance the upconversion from visible (VIS) to ultraviolet C (UVC) in order to achieve improved bactericidal efficacy [3]. One potential approach entails investigating the structure- optical properties correlations through the utilization of High-resolution photoluminescence, employing lanthanide dopants as a probe.

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CORRELATION BETWEEN MICROSTRUCTURE AND ELECTRIC PROPERTIES OF Li-Nb-Ti-O CERAMICS

Radoš R. Raonić^a, Dalibor L. Sekulić^b, Svetlana R. Lukić-Petrović^a, Tamara B. Ivetić^a

^a*University of Novi Sad, Faculty of Sciences, Department of Physics, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia, rados.raonic@df.uns.ac.rs*

^b*University of Novi Sad, Faculty of Technical Sciences, Department of Power, Electronic and Telecommunication Engineering, Trg Dositeja Obradovića 6, 21000 Novi Sad, Serbia*

In this study we investigated the relationship between electrical properties and microstructure of lithium-niobium-titanium-oxide (Li-Nb-Ti-O) ceramics by changing the concentration of ZnO as a modifier and/or using polyvinyl alcohol as a binder during the synthesis by mechanochemical solid-state reaction method. The electrical properties of Li-Nb-Ti-O ceramics, which can be tailored by the changing the concentration of the constituent components and/or small additions of modifiers, make them a promising material for various applications in microelectronic devices. In addition, lowering their sintering temperature during synthesis places them to the group of suitable candidates for low-temperature co-fired ceramics (LTCC) technology. A microstructure composed of rod- and plate-shaped particles, showing the typical morphology of the *M*-phase group of Li-Nb-Ti-O compounds, was observed in scanning electron microscopy (SEM) images. Further, complex impedance spectroscopy analysis was used to determine a possible conduction mechanism which was correlated with the resulting microstructure.

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SURFACE MODIFICATION OF TITANIUM SCAFFOLD FOR RESTORATION OF BONE DEFECTS

Marija Milivojević^a, Vesna Kojić^b, Rada Petrović^c, Đorđe Janačković^c

^a*Innovation Center of Faculty of Technology and Metallurgy, Karnegijeva 4, Belgrade, Serbia, mmilivojevic@tmf.bg.ac.rs*

^b*Faculty of Medicine, Oncology Institute of Vojvodina, University of Novi Sad, Sremska Kamenica, Serbia, vesna.kojic@sbb.rs*

^c*Faculty of Technology and Metallurgy, Karnegijeva 4, Belgrade, Serbia, radaab@tmf.bg.ac.rs, nht@tmf.bg.ac.rs*

The management of large bone defects, conventionally addressed through bone graft transplantation, has experienced significant advancements within the field of biomaterial engineering. Custom-designed 3D-printed macroporous titanium (Ti) scaffolds have emerged as a highly promising therapeutic approach. These scaffolds offer a dual advantage by providing mechanical support to the bone and a pore architecture conducive to bone tissue ingrowth, promoting osseointegration. However, the bioinert nature of the widely used Ti6Al4V alloy surface presents a limitation for optimal cell growth and mineral matrix deposition. Additionally, leaching of the ions from the alloy in the organism upon implantation can cause adverse effects.

To address these challenges related to Ti6Al4V bioinert surface and impact of alloy ion leakage on cytocompatibility, we introduced a surface modification approach by coating the scaffold with bioactive glasses and hydroxyapatite. This modification not only reduced corrosion but also provided a bioactive surface.

The 3D-printed macroporous scaffolds, fabricated using Electron Beam Melting (EBM) technology, underwent surface modification through dipcoating. The resulting three-layer coating consisted of two graded bioactive glasses (6P64 and 6P57) and hydroxyapatite, which had been characterized using Scanning Electron Microscopy (SEM) and Fourier Transform Infrared Spectroscopy (FT-IR). Subsequently, the coating was annealed at 850°C in an inert atmosphere and subjected to further characterization. SEM was used to observe the coating surface and cross-sections, and Energy-Dispersive X-ray Spectroscopy (EDX) was employed for elemental mapping analysis. Ion leakage from both the uncoated Ti sample and the coated samples was analyzed using Inductively Coupled Plasma Optical Emission Spectrometry (ICP-OES). The cytocompatibility of the scaffolds was evaluated using two human cell lines, L929 and MRC5, through the MTT test.

The results demonstrated that coating with bioactive glasses effectively reduces the leakage of vanadium ions from the alloy. SEM and EDX analyses revealed a continuous layer of melted glass on the alloy's surface, which likely acted as a barrier to ion release from the alloy. Furthermore, the metabolic activity of cells significantly improved in the coated scaffolds compared to the bare Ti scaffold for both tested cell lines. These findings suggest that coating of titanium-based macroporous scaffolds with bioactive ceramics enhances cellular response and holds potential applications in orthopedics.

**SYNTHESIS AND HIGH-TEMPERATURE / HIGH-PRESSURE
EXPOSURE OF COMPOSITIONALLY COMPLEX ROCK-SALT-TYPE
TRANSITIONAL METAL (CARBO)NITRIDES**

Dharma Teja Teppala^a, Shrikant Bhat^b, Leonard Keil^a, Jan Bernauer^a, Johannes Peter^c, Hans-Joachim Kleebe^c, Emanuel Ionescu^{a,d}

^a*Institute for Material Science, Technical University of Darmstadt, 64287 Darmstadt, Germany*

^b*Photon Science, DESY, 22607 Hamburg, Germany*

^c*Institute for Applied Geosciences, Technical University of Darmstadt, 64287 Darmstadt, Germany*

^d*Fraunhofer IWKS, Brentanostrasse 2a, 63755 Alzenau, Germany*

Transitional metal carbides and nitrides, especially of group IV and V metals, are well known in the ceramic field due to their good thermal, electrical properties, high hardness, and high temperature stability making them useful in applications that require high hardness and resistance to various corrosive atmospheres. There is abundant thermodynamic data available on binary transitional metal carbides and nitrides, such as P-T phase diagram, thermal expansion, Debye temperature and physical parameters, e.g., elastic moduli; while this is rather not the case for ternary and other high complex compositions.

Transitional metal nitrides, especially those of group IV metals, are known to form simple, high symmetry structures at ambient conditions, i.e., rock salt. However, at high pressure and temperatures, the metal nitrides were observed to undergo phase transition and these thermodynamically stable high-pressure phases were observed or predicted to be denser, harder with distinct properties compared to that of the ambient condition phase.

In the present work, two carbonitride-based complex compositions i.e. $(\text{Ti}_{0.2}\text{Zr}_{0.2}\text{Hf}_{0.2}\text{Nb}_{0.2}\text{Ta}_{0.2})\text{N}_x\text{C}_{1-x}$ and $(\text{V}_{0.2}\text{Nb}_{0.2}\text{Ta}_{0.2}\text{Mo}_{0.2}\text{W}_{0.2})\text{N}_x\text{C}_{1-x}$ were synthesized via a non-oxidic sol-gel process using the respective metal amido complexes and ammonia followed by a thermal ammonolysis at 1000 °C. The obtained phase-pure carbonitrides were structurally characterized by X-ray diffraction and electron microscopy and then considered for performing experiments under extreme conditions i.e pressures up to 20 GPa and temperatures as high as 1900°C. The experiments were performed in the large volume press facility at the beam line P61B DESY.

The in-situ x-ray diffraction study during the high-temperature high-pressure treatment revealed that the rock salt structure of the compositionally complex carbonitrides was stable under the conditions of exposure and allowed to quantify for the first time some basic physical parameters thereof, e.g., thermal expansion and bulk modulus, which were calculated by using 3rd order Birch Murnaghan equation of state.

Eu³⁺-ACTIVATED RED AND DEEP-RED-EMITTING PHOSPHOR FOR PLANT GROWTH LED APPLICATION

Bojana Milićević, Mina Medić, Zoran Ristić, Katarina Milenković, Željka Antić, Miroslav D. Dramićanin

Centre of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, P.O. Box 522, Belgrade, bojana.milicevic85@gmail.com

The light-emitting-diode (LED) is revolutionizing general illumination with the promise of enormous energy savings when widespread adoption occurs. However, current LED technologies for plant cultivation are less developed compared to LEDs for general lighting. As LEDs continue to grow in the diversity of package designs, their luminescent features and performance are mainly influenced by the phosphors used in the packages.

Eu³⁺-activated inorganic phosphors are traditionally used for general lighting and display because they usually emit either intense orange ($^5D_0 \rightarrow ^7F_1$) or red ($^5D_0 \rightarrow ^7F_2$) light whose wavelength is shorter than 630 nm. Nevertheless, when Eu³⁺ occupies the lattice position in the non-inverted center of low symmetry, the possibility of $^5D_0 \rightarrow ^7F_4$ transitions increases, resulting in far-red emissions (> 700 nm) that may be more intense than orange and red ones. Herein, a novel Eu³⁺-activated phosphor, Sr₂GdF₇:Eu³⁺, is produced with the conventional hydrothermal technique. An efficient complexing agent was used in a typical synthesis to improve crystal seed dispersibility, produce metal complexes, and prevent particle aggregation. This technique yields products with small particles of approximately 30 nm. Differing from other Eu³⁺-activated phosphors, the $^5D_0 \rightarrow ^7F_2$ and $^5D_0 \rightarrow ^7F_4$ transition of Eu³⁺ in this host are dominant, and red and deep red emissions are balanced. Such special features of Eu³⁺ luminescence mainly meet the need for phytochrome photoreceptors (PFR and PR) in plants. The long lifetime (approximately 13 ms) is caused by the crystal structure and low phonon energy of Sr₂GdF₇ that lead to less efficient non-radiative processes.

Therefore, Eu³⁺-activated Sr₂GdF₇ is suitable for LEDs that may offer several benefits, including increased yields, earlier flowering, faster root growth/germination, better control of plant growth, and more economical use of arable land.

SYNTHESIS AND LUMINESCENCE PROPERTIES OF CORE-SHELL CsY₂F₇:Eu NANOPARTICLES

Katarina Milenković, Ivana Zeković, Bojana Milićević, Vesna Đorđević, Miroslav Dramićanin
*Center of Excellence for Photoconversion, Vinča Institute of Nuclear Sciences – National
Institute of the Republic of Serbia, University of Belgrade, Serbia,
katarina.milenkovic@vin.bg.ac.rs*

Core-shell nanoparticles are a class of nanomaterials which have become a subject of growing interest due to their fascinating characteristics. Those nanoparticles are consisted of inner material- core and outer material- shell, which allow for exact control over their properties and capabilities.

The CsY₂F₇ is a member of the expanding class of rare earth fluoride nanomaterials. Because of isostructural exchange of yttrium ions with other trivalent rare earths, material can exhibit a variety of luminous properties.

Nanoparticles of CsY₂F₇ doped with 25% Eu³⁺ ions are successfully synthesized using microwave assisted solvothermal synthesis. CsY₂F₇:25%Eu nanophosphors are coated by silica (SiO₂), sodium hexametaphosphate (NaHMP) and polyacrylic acid (PAA) via precipitation method and by cesium yttrium fluoride (CsY₂F₇) via microwave assisted solvothermal method. X-ray diffraction, Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM) and photoluminescence spectroscopy were applied to characterize these CsY₂F₇:Eu@SiO₂, CsY₂F₇:Eu@PAA, CsY₂F₇:Eu@NaHMP and CsY₂F₇:Eu@CsY₂F₇ core-shell structures.

All prepared core-shell structures of CsY₂F₇:25%Eu exhibit the same orthorhombic symmetry with Pnna (52) space group crystallization as the original CsY₂F₇ nanoparticles. Successful coating of core nanoparticles has been confirmed by FTIR spectra. SEM of CsY₂F₇:25%Eu@SiO₂ and CsY₂F₇:25%Eu@PAA samples reveals that several core nanoparticles were aggregated by shell material, whereas this phenomenon is not observed for NaHMP and CsY₂F₇ shells. The emission spectra of CsY₂F₇:25%Eu nanoparticles show typical Eu³⁺ transitions, with excitation wavelengths of 393 nm resulting in emissions at 579, 593, 612, 651, and 699 nm, corresponding to ⁵D₀ to ⁷F_J (J= 0, 1, 2, 3, 4, respectively). The intensity of the characteristic emissions varied after coating the nanoparticles with different shells, while the emissions remained at the same wavelengths. CsY₂F₇:25%Eu@NaHMP becomes the most promising core-shell nanoparticle, with enhanced red emission peaking at 612 nm.

The unique structure and enhanced properties of core-shell nanoparticles have made them useful for a wide range of applications, including optoelectronics, sensing, and biomedicine, where CsY₂F₇:25%Eu@NaHMP nanoparticles with improved luminescence can be used.

PENETRATION AIRCRAFT BOMB BLU-109E MATERIAL SELECTION

Nemanja Deura, Boško Božilović, Srećko Nijemčević
Vlatacom Institute, Blvd. Milutina Milankovica 5, Belgrade, Serbia,
nemanja.deura@vlatacom.com

This paper describes the process of designing and testing the aircraft bomb vPRAB-1000-9 (Hereinafter BLU-109E) with special emphasis on the choice of materials and testing methods to which the materials and weapons are subjected so that the weapons meet both the criteria of military standards and functional and operational characteristics.

Aircraft penetration bomb BLU-109E is a penetration aircraft ballistic bomb of special purpose. It is intended for annihilation and neutralization of reinforced objects, located on the surface, buried under the ground or sheltered behind rocky terrain. The bomb realizes its effect by penetrating through the object protective walls and, after penetration, by a controlled detonation of the explosive charge, primarily by a shock wave and secondarily by the fragmentation of its steel casing.

Due to the purpose of this weapon, in addition to the design of the aircraft bomb itself, it is essential to choose the appropriate material from which the bomb is manufactured.

The raw material used in the manufacture of the parts of this aircraft bomb is subjected to chemical and mechanical tests before the manufacture of the parts in order to confirm its declared characteristics.

In addition, every part that is manufacture, of which the aerial bomb is composed, as well as the bomb itself, is subjected to certain static and dynamic tests, as well as testing the environmental effects that the weapon may experience during its lifespan.

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