

The Serbian Society for Ceramic Materials  
Institute for Multidisciplinary Research (IMSI), University of Belgrade  
Institute of Physics, University of Belgrade  
Center of Excellence for the Synthesis, Processing and Characterization of  
Materials for use in Extreme Conditions "CEXTREME LAB" - Institute of  
Nuclear Sciences "Vinča", University of Belgrade  
Faculty of Mechanical Engineering, University of Belgrade  
Center for Green Technologies, Institute for Multidisciplinary Research,  
University of Belgrade  
Faculty of Technology and Metallurgy, University of Belgrade  
Faculty of Technology, University of Novi Sad

A microscopic image showing a dense collection of small, rounded, light-colored particles, likely ceramic grains, against a darker background. The particles are uniform in size and shape, creating a textured, granular appearance.

# PROGRAMME and the BOOK of ABSTRACTS

## 5CSCS-2019

5<sup>th</sup> Conference of  
the Serbian Society for Ceramic Materials  
June 11-13.2019. Belgrade Serbia

Edited by:  
**Branko Matović**  
**Zorica Branković**  
**Aleksandra Dapčević**  
**Vladimir V. Srdić**

Programme and Book of Abstracts of The Fifth Conference of The Serbian Society for Ceramic Materials **publishes abstracts from the field of ceramics, which are presented at international Conference.**

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***Publisher***

Institute for Multidisciplinary Research, University of Belgrade

Kneza Višeslava 1, 11000 Belgrade, Serbia

***For Publisher***

Prof. Dr Sonja Veljović Jovanović

***Printing layout***

Vladimir V. Srdić

***Press***

Faculty of Technology and Metallurgy, Research and Development Centre of Printing Technology, Karnegijeva 4, Belgrade, Serbia

***Published:*** 2019

***Circulation:*** 150 copies

CIP - Каталогизacija у публикацији - Народна библиотека Србије, Београд

666.3/.7(048)

66.017/.018(048)

**DRUŠTVO za keramičke materijale Srbije. Konferencija (5 ; 2019 ; Beograd)**

Programme ; and the Book of Abstracts / 5th Conference of The Serbian Society for Ceramic Materials, 5CSCS-2019, June 11-13, 2019, Belgrade, Serbia ; [organizers] The Serbian Society for Ceramic Materials ... [et al.] ; edited by Branko Matović ... [et al.]. - Belgrade : Institute for Multidisciplinary Research, University, 2019 (Beograd : Faculty of Technology and Metallurgy, Research and Development Centre of Printing Technology). - 139 str. : ilustr. ; 24 cm

Tiraž 150. - Str. 6: Welcome message / Branko Matovic. - Registar.

ISBN 978-86-80109-22-0

a) Керамика - Апстракти

b) Наука о материјалима - Апстракти

c) Наноматеријали - Апстракти

COBISS.SR-ID 276897292

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Edited by:  
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**Vladimir V. Srdić**

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## WELCOME MESSAGE

The 5<sup>th</sup> Conference of the Serbian Society for Ceramic Materials: 5CSCS-2019 aims to review the knowledge, experience and share new ideas among the professionals, industrialists and students from research areas of ceramic materials and by taking an active part in discussions and technical sessions at the conference. The conference provides exhibitor booths for the companies and the institutions to showcase their services, products, innovations, innovative ideas and research work & results.

The conference includes all aspects of ceramics: modelling, synthesis, properties, processing and applications of bulk, films, powders, nanomaterials, composites providing a platform for academic exchange among participants from universities, institutes, companies around the region in the field of ceramics research as well as to explore a new direction for future development. The conference has an elemental feature to the distinguished motive speakers, plenary speeches, young investigators, poster presentations, oral presentations, technical workshop, and scientific sessions.

The conference is hosted and organized by the Serbian Society for Ceramic Materials, and co-organized by the Institute for Multidisciplinary Research - University of Belgrade, Center of Excellence for the Synthesis, Processing and Characterization of Materials for use in Extreme Conditions “CEXTREME LAB” - Institute of Nuclear Sciences “Vinča” - University of Belgrade, Institute of Physics - University of Belgrade, Faculty of Mechanical Engineering - University of Belgrade, Center for Green Technologies of the Institute for Multidisciplinary Research - University of Belgrade, Faculty of Technology and Metallurgy - University of Belgrade, Faculty of Technology - University of Novi Sad.

We are grateful for the support of the Ministry for education, science and technological development of the Republic of Serbia. We would also like to express our sincere thanks to the conference organizers, session chairs, presenters, exhibitors and all the conference attenders for their efforts and enthusiastic support in this exciting time in Belgrade. I look forward to meeting you and interacting with you at Conference.

Branko Matovic,  
President of the Serbian Society for Ceramic Materials



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# PROGRAMME

## Day 1. Tuesday - June 11, 2019

**08.00-09.00 Registration**

**09.00-09.30 Opening ceremony and welcome addresses**

**09.30-10.00 Cocktail**

### **Plenary lecture**

Chair: Yuri Rostovtsev, Xavier Rocquefelte

**10.00-10.30 Plenary lecture, PL-1**

J. Christian Schön, *(BIO)MOLECULES, IN VACUUM AND ON SURFACES: WHAT DO THE ENERGY LANDSCAPES OF SUCH MATERIALS TELL US?*

### **Session 1: Ceramic Powders, Characterization and Processing**

Chair: Vladimir Srđić, Jasminka Popović

**10.30-10.50 Invited lecture, I-1**

Jasminka Popović, *2D LAYERED HYBRID ORGANIC-INORGANIC PEROVSKITES FOR ADVANCED LIGHT EMITTING APPLICATIONS*

**10.50-11.10 Invited lecture, I-2**

Anna Gubarevich, *COMBUSTION SYNTHESIS OF MAX PHASE SOLID SOLUTIONS IN Ti-Zr-Al-C AND Ti-Zr-Si-C SYSTEMS*

**11.10-11.30 Invited lecture, I-3**

Vesna Srot, *NANOSCALE CHARACTERIZATION OF INTERFACES IN FUNCTIONAL MATERIALS*

**11.30-11.50 Invited lecture, I-4**

Sonja Smiljanić, *FROM GLASS TO GLASS-CERAMIC*

**11.50-12.10 Coffee break**

### **Session 1: Ceramic Powders, Characterization and Processing**

Chair: Vladimir Srđić, Jasminka Popović

**12.10-12.30 Invited lecture, I-5**

Dušan Bučevac, *YAG:Ce,Pr YELLOW-EMITTING PHOSPHOR WITH ENHANCED RED EMISSION FOR WHITE LEDS*

**12.30-12.45 Oral presentation, O-1**

Milica Počuča-Nešić, *MECHANOCHEMICAL vs. CHEMICAL SYNTHESIS IN THE PREPARATION OF  $Y\text{MnO}_3$  CERAMIC MATERIALS*

**12.45-13.00 Oral presentation, O-2**

Ivana Milenković, *COATING OF CERIUM OXIDE NANOPARTICLES WITH DIFFERENT CARBOHYDRATES*

**13.00-13.15 Oral presentation, O-3**

Milan Vasić, *RELEVANT PROPERTIES OF GREEN SELF COMPACTING CONCRETE*

**13.15-14.30 Lunch break**

**13.15-14.30 Poster Session 1 (Posters P1 – P34)**

**Session 2: High Temperature Phenomena, Sintering, Microstructure Design and Mechanical Properties**

Chair: Žaklina Burghard, Miladin Radović

**14.30-14.50 Invited lecture, I-6**

Žaklina Burghard, *STRUCTURING OF HIGHLY POROUS MECHANICALLY STABLE SCAFFOLDS*

**14.50-15.10 Invited lecture, I-7**

Peter Tatarko, *DEVELOPMENT OF ULTRA-HIGH TEMPERATURE CERAMICS BY FIELD ASSISTED SINTERING TECHNOLOGY*

**15.10-15.30 Invited lecture, I-8**

Miladin Radović, *ALUMINA FORMING MAX PHASES: CURRENT STATUS AND FUTURE PERSPECTIVES*

**15.30-15.50 Invited lecture, I-9**

Tetiana Prikhna, *MAX MATERIALS AND COATINGS STABLE IN OXIDIZING AND HYDROGEN ATMOSPHERES AT HIGH TEMPERATURES*

**15.50-16.10 Invited lecture, I-10**

Aleksander Rečnik, *TOPOTAXIAL PHASE TRANSFORMATIONS AND TWINNING OF RUTILE*

## Day 2. Wednesday - June 12, 2019

### Plenary lecture

Chair: Malgorzata Makowska-Janusik, Dejan Zagorac

#### 09.00-09.30 Plenary lecture, PL-2

Klaus Doll, *STRUCTURE-PROPERTY RELATIONSHIPS FROM ELECTRONIC STRUCTURE CALCULATIONS*

### Session 3: Computing in Materials Science

Chair: Malgorzata Makowska-Janusik, Dejan Zagorac

#### 09.30-09.50 Invited lecture, I-11

Yuri Rostovtsev, *MATERIALS WITH EXCITED QUANTUM COHERENCE: FROM PLASMONICALLY INDUCED TRANSPARENCY TO QUANTUM CORRELATION*

#### 09.50-10.10 Invited lecture, I-12

Malgorzata Makowska-Janusik, *NANOSIZED SEMICONDUCTING MATERIALS - THEIR PROPERTIES AND APPLICATIONS – THEORETICAL APPROACH*

#### 10.10-10.30 Invited lecture, I-13

Xavier Rocquefelte, *THEORETICAL INVESTIGATION OF MAGNETIC AND MULTIFERROIC PROPERTIES*

#### 10.30-10.45 Oral presentation, O-4

Dejan Zagorac, *FIRST-PRINCIPLES INVESTIGATIONS OF ZnO/ZnS MIXED COMPOUNDS, POLYTYPISM AND (HETERO)STRUCTURES*

#### 10.45-11.00 Oral presentation, O-5

Jelena Zagorac, *FIRST PRINCIPLE INVESTIGATION OF  $Al_{1-x}B_xN$  SOLID SOLUTION*

#### 11.00-11.15 Oral presentation, O-6

Rühl Stephan, *THE INORGANIC CRYSTAL STRUCTURE DATABASE (ICSD)*

#### 11.15-11.40 Coffee break

### Session 4: Ceramic Composites, Membranes and Multimaterials

Chair: Ravi Kumar, Branko Matović

#### 11.30-11.50 Invited lecture, I-14

Ravi Kumar, *PLASMON ENHANCED VISIBLE LIGHT PHOTOCATALYTIC ACTIVITY IN POLYMER-DERIVED TIN/SI-O-C-N NANOCOMPOSITES*

#### 11.50-12.10 Invited lecture, I-15

Carmen Galassi, *MICROSTRUCTURE CONTROL IN MULTIFERROIC COMPOSITES*

#### 12.10-12.30 Invited lecture, I-16

Sanja Vranjes-Đurić, *RADIOLABELLED NANOMATERIALS DESIGNED FOR APPLICATION IN MEDICINE*

**12.30-12.50 Invited lecture, I-17**

Nikola Dudukovic, *3D PRINTING OF MULTIMATERIAL GLASS AND CERAMIC OPTICS*

**12.50-13.10 Invited lecture, I-18**

Andreja Gajović, *PREPARATION AND MECHANICAL PROPERTIES OF POROUS ZIRCONIA/CALCIUM PHOSPHATES CERAMIC COMPOSITES*

**13.10-13.25 Oral presentation, O-7**

Victor Fruth, *MULTIFUNCTIONAL COMPOSITE COATINGS WITH SELF-CLEANING AND ANTIMICROBIAL PROPERTIES CONTAINING OXIDE NANOPOWDERS*

**13.25-13.40 Oral presentation, O-8**

András Kovács, *SYNTHESIS AND QUANTIFICATION OF KAOLINITE NANOSCROLLS*

**13.40-14.30 Lunch break**

**13.40-14.30 Poster Session 2 (Posters P35 – P59)**

**15.00-18.00 Excursion**

**20.30-01.00 Conference dinner**

## Day 3. Thursday - June 13, 2019

### Session 5: Electro and Magnetic Ceramics

Chair: Goran Branković, Slavko Bernik

**09.00-09.20 Invited lecture, I-19**

Barbara Malić, *RELAXOR FERROELECTRIC CERAMICS FOR ELECTROCALORIC COOLING: PROCESSING CHALLENGES AND POSSIBLE APPLICATIONS*

**09.20-09.40 Invited lecture, I-20**

Goran Branković, *EXPERIMENTAL EVIDENCE OF ELECTRO-MECHANICAL COUPLING IN CUBIC YSZ*

**09.40-10.00 Invited lecture, I-21**

Slavko Bernik, *ENGINEERING OF DEFECTS AND THERMOELECTRIC PROPERTIES OF ZnO CERAMICS*

**10.00-10.20 Invited lecture, I-22**

Floriana Craciun, *DIELECTRIC AND ANELASTIC SPECTROSCOPY: A POWERFUL COMBINED TOOL FOR CHARACTERIZING MULTIFUNCTIONAL CERAMICS*

**10.20-10.40 Invited lecture, I-23**

Dejan Djokić, *VARIABLE RANGE HOPPING MECHANISM OF CARRIER TRANSPORT IN BiFeO<sub>3</sub> NANO-PARTICLES REVEALED VIA RAMAN SCATTERING TECHNIQUE*

**10.40-11.00 Invited lecture, I-24**

Pavle Premović, *ELECTRON SPIN RESONANCE STUDIES OF NATURAL KAOLINITES: A BRIEF REVIEW*

**11.00-11.30 Coffee break**

### Session 5: Electro and Magnetic Ceramics

Chair: Zorica Branković, Barbara Malić

**11.30-11.45 Oral presentation, O-9**

Branko Matović, *PREPARATION OF Ag DOPED CERIA CERAMICS*

**11.45-12.00 Oral presentation, O-10**

Nebojša Nikolić, *FORMATION OF METAL POWDERS ELECTROLYSIS: COMPARISON OF MORPHOLOGICAL AND CRYSTALLOGRAPHIC CHARACTERISTICS*

**12.00-12.15 Oral presentation, O-11**

Milan Žunić, *SPIN-COATING DEPOSITION OF DENSE BaZr<sub>0.7</sub>Pr<sub>0.1</sub>Y<sub>0.2</sub>O<sub>3-δ</sub> ELECTROLYTE THICK FILMS ON NI-BASED ANODES FOR IT-SOFCs*



**12.15-12.30 Oral presentation, O-12**

Katarina Vojisavljević, *HUMIDITY SENSOR BASED ON MESOPOROUS SnO<sub>2</sub> FABRICATED VIA NANOCASTING TECHNIQUE*

**12.30-12.45 Oral presentation, O-13**

Andrea Nesterović, *PROCESSING OF Bi<sub>0.5</sub>Na<sub>0.5</sub>TiO<sub>3</sub> BASED PIEZOELECTRIC CERAMICS*

**12.45-13.00 Oral presentation, O-14**

Jiangguli Peng, *THE INTERPLAY OF PHASES, STRUCTURAL DISORDER AND DIELECTRIC BEHAVIOR IN Al DOPED BiFeO<sub>3</sub>-BaTiO<sub>3</sub> CERAMICS*

**13.00-14.30 Lunch break**

**13.00-14.30 Poster Session 3 (Posters P60 – P74)**

**Session 6: Traditional Ceramics**

Chair: Tatjana Volkov-Husović, Eniko Volceanov

**14.30-14.50 Invited lecture, I-25**

Tatjana Volkov Husović, *TRADITIONAL CERAMICS: PAST, PRESENT AND FUTURE*

**14.50-15.10 Invited lecture, I-26**

Enikő Volceanov, *ECO-CERAMICS FOR BLAST MITIGATION*

**15.10-15.30 Invited lecture, I-27**

Claudio Ferone, *SELF-SUPPORTING ZEOLITES BY GEOPOLYMER GEL CONVERSION. EVALUATION FOR WATER SOFTENING APPLICATIONS*

**15.30-15.50 Invited lecture, I-28**

Gábor Mucsi, *CONTROLLING THE GEOPOLYMERIZATION REACTIONS BY MECHANICAL ACTIVATION OF SECONDARY RAW MATERIALS*

**15.50-16.05 Oral presentation, O-15**

Florica Matau, *TEMPERING RECIPES OF THE CHALCOLITHIC POTTERY. CASE STUDIES FROM EASTERN ROMANIA*

**16.05-16.30 Closing ceremony**



PL-1

**(BIO)MOLECULES, IN VACUUM AND ON SURFACES: WHAT  
DO THE ENERGY LANDSCAPES OF SUCH MATERIALS  
TELL US?**

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At the beginning of chemistry as a science, a division was established into organic and inorganic chemistry, each realm with its own special concerns and methodologies, which has been surprisingly persistent. But in recent years there has been an increased interest in studying the behavior of systems or materials that partake in both realms, driven by fields as diverse as medicine, environmental science, organic electronics and sensor technology, catalysis, or flexible materials. Typically, a crucial element of such systems or hybrid materials are interfaces between biomolecules or, more generally, organic or metal organic molecules, and some inorganic metallic or ceramic surface. Selecting the right combinations of molecule and inorganic substrate allows a fine-tuning of the physical and chemical properties - both static and dynamic - of such a system, to a much larger degree than is possible for bulk organic or inorganic materials. On the other hand, it is considerably more difficult to analyze the atomic arrangements and atom/molecule level processes in such hybrid systems, and thus theoretical tools are needed to determine or even predict the (possible) structures present in the chemical system, both in equilibrium and in non-equilibrium situations. Similar to nanoparticles, the stability of a given interface or arrangement of (bio)molecules on a surface are usually considerably lower than one is used from bulk materials. Both the investigation of the wide range of possible structures in the system and the analysis of their stability rely on the study of the energy landscape of the system: the determination of the minima on the landscape and the generalized barriers separating them. Furthermore, the possible design of hybrid materials e.g. via molecule by molecule placement on a surface or insertion into a layered matrix, relies on information about the properties of the corresponding energy landscape.

In this presentation, we explore applications of energy landscapes to (bio)molecule-inorganic systems, ranging from the study of individual molecules, in vacuum and on surfaces, to periodic multi-molecular arrangements on surfaces.

PL-2

## STRUCTURE-PROPERTY RELATIONSHIPS FROM ELECTRONIC STRUCTURE CALCULATIONS

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Electronic structure calculations based on density functional theory are nowadays widely used to complement the experiment. One research area is predicting and optimising structures. Closely related is the calculation of properties for these structures. This allows to establish relationships between the structure of a material and its properties, and to work out guidelines to tune material properties.

BaS crystallises in a rock salt structure at ambient pressure, and in a CsCl structure at high pressure. Recently, various other modifications have been studied, and their properties such as band structures and especially band gaps, but also elastic properties are discussed. [1,2]

Infrared and Raman spectra can nowadays be simulated and are in very good agreement with experimental data. Moreover, simulation can be used to identify peaks with little intensity and which are thus difficult to find in the experiment. Results are shown for systems such as Mn<sub>3</sub>O<sub>4</sub> bulk [3], Cr<sub>2</sub>O<sub>3</sub> bulk [4], and for bulk, surfaces and nanotubes of BeS [5] and Y<sub>2</sub>O<sub>3</sub>.

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I-1

## 2D LAYERED HYBRID ORGANIC-INORGANIC PEROVSKITES FOR ADVANCED LIGHT EMITTING APPLICATIONS

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Two dimensional (2D) perovskites or Ruddlesden-Popper (RP) perovskites, are currently attracting lots of attention for light emitting device (LED) applications [1]. These 2D materials are described by general formula  $R_2A_{n-1}B_nX_{3n+1}$ , where R is the

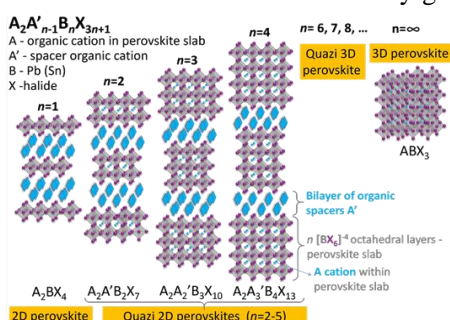


Figure 1. Structure of 2D perovskites

2D perovskites represent an excellent working platform, extremely versatile and highly tailorable, because properties can be tuned not only by the choice of organic cations (A and A') and halide anions, but also by changing  $n$  [1,2]. One interesting feature of 2D perovskites is the fact that the optoelectronic properties (both band gap and excitation binding energy) are highly dependent on the degree of quantum confinement, which is mainly dominated by thickness  $n$  of inorganic slab, which means the color can easily be tuned, depending on chosen  $n$ . Tuning the band gap by controlling the  $n$  indeed works perfectly for the exfoliated single crystals of these materials; the problem, which is still unsolved, relates to the fact that thin films or powders typically consist of a mixture of phases with different  $n$ . Achieving more control over phase composition is prerequisite for further development of 2D-perovskite-based LEDs, thus, we try to achieve phase composition control by different approaches of rational structural design. This talk will address the structural features and optical properties of  $n=2$  perovskite materials with utilization of mixed organic cations in organic layer. Additionally, the alternative synthetic approaches for the preparation of  $n=4$  perovskites with bright emission will be discussed.

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I-2

## COMBUSTION SYNTHESIS OF MAX PHASE SOLID SOLUTIONS IN TI-ZR-AL-C AND TI-ZR-SI-C SYSTEMS

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MAX phases, ternary inorganic compounds with composition  $M_{n+1}AX_n$  (M is a transition metal, A is an element of A-group, X is carbon or nitrogen, and n is typically 1 to 3), have hexagonal crystal lattice and show specific nanolaminated structure [1]. MAX phases have been attracting an increasing attention due to a unique combination of properties, which are intermediate between metals and ceramics [1,2]. Zirconium-based MAX phases represent a special interest for application in nuclear energy field due to the small neutron cross-section of zirconium. However, synthesis of pure zirconium MAX phases such as  $Zr_3AlC_2$  or  $Zr_2AlC$  is very difficult [3], and no MAX phase in Zr-Si-C has been reported yet. From the other side, formation of solid solutions in MAX phase family can be an effective approach to find new compositions with desired characteristics.

In the present work, MAX phase solid solutions in Ti-Zr-Al-C and Ti-Zr-Si-C systems were synthesized by combustion synthesis method, which has merits of simplicity, high time and energy efficiency. Elemental powders were mixed, pressed into pellets and ignited using tungsten filament under Ar atmosphere. Propagation of combustion reaction was confirmed for all compositions studied.

In Ti-Zr-Al-C system, the best result was achieved for  $ZrTi_2AlC_2$  composition with the yield of MAX phase determined using Rietveld refinement of XRD data about 90 %. The lattice parameters for  $ZrTi_2AlC_2$  were consistent with the theoretical values from [4]. Increasing proportion of Zr to Ti led to lowering the yield of MAX phase, while the crystal lattice parameters *a* and *c* increased with the content of Zr. Formation of MAX phase solid solutions in Ti-Zr-Si-C system was found for the first time. The yield of  $Zr_xTi_{3-x}SiC_2$  MAX phase solid solutions considerably decreased with increasing of Zr content.

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I-3

## NANOSCALE CHARACTERIZATION OF INTERFACES IN FUNCTIONAL MATERIALS

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The microstructure and local chemistry are dominating the physical, chemical and mechanical properties of advanced functional materials. With the latest technical and methodological developments scanning transmission electron microscopy (STEM) entered a completely new area, enabling studies of fascinating phenomena at the nanoscale. Several different types of functional materials have been investigated: (i) ultra-thin films in functional complex oxides, (ii) man-made bio-inspired multilayered functional materials, (iii) natural composite functional materials.

- (i) High quality ultra-thin  $\text{NdBa}_2\text{Cu}_3\text{O}_7$  (NBCO) films deposited on  $\text{SrTiO}_3$  (STO) substrates have been examined. In NBCO, the Cu atoms are located in the  $\text{CuO}_2$  planes and in parallel CuO chains, with Nd atoms positioned between the planes and the chains. Physical properties of NBCO can be drastically influenced due to oxygen content fluctuations, where the charge balance between the planes and the chains has high influence on  $T_c$  [1]. We have used atomically resolved STEM imaging to study the local cation and anion sub-lattices and their distortions. The chemical identity of NBCO films and NBCO/STO interfaces has been investigated by a combination of atomically resolved imaging and analytical methods [2].
- (ii) Unique and highly complex architectures of organic-inorganic hybrid materials have been a great inspiration for modern man-made materials design. For our study, M13 wild-type phages have been used as scaffolds for assembling layer-by-layer structures consisting of alternating M13 phages and ZnO layers. Nanoscale investigations have revealed homogeneous organic/inorganic multilayered structures with limited interpenetration at the M13 phages-ZnO interfaces [3].
- (iii) Constantly growing rodent teeth are a perfect example of optimally designed organic-inorganic nanoarchitectures composed of simple and closely linked compounds. We exposed a chemically diverse Fe-enriched surface layer (Fe-SL) that is covering pigmented enamel. Chemical analysis demonstrated the existence of an Fe-SL with Fe in predominantly 3+ valence state. The present results reveal close interaction between ideally tailored architectures and materials' functionality in natural complex materials [4].

*Acknowledgment:* This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823717 – ESTEEM3.

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I-4

## FROM GLASS TO GLASS-CERAMIC

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Glass ceramics is a partially crystalline material obtained by controlled crystallization of glass. Glass-ceramics can be formed from the bulk glass through the processes of controlled nucleation and crystallization by adequate heat treatment. An alternative method for glass-ceramic production is the sintering of the glass powder. Producing high-quality parent glass is an important step in obtaining glass-ceramic materials. In order to obtain flawless glass or to obtain glass-ceramic material with specific properties, it is necessary to understand the crystallization characteristics of the glass, such as the mechanism of crystallization, the temperature range of nucleation and the growth of crystals [1].

During the heat treatment of the bulk glass samples crystalline phase is formed. The composition of crystalline phase and its microstructure determine improved thermal, chemical, optical, electrical or mechanical properties in relation to the starting glass. Separation of certain phases, their phase composition and microstructure, therefore, do not depend only on the selected composition of glass, but also on the heat treatment conditions. The important advantage of glass-ceramics is the ability to form different microstructures depending on the heat treatment and the composition of the glass.

When applying glass powder sintering, densification and crystallization processes are simultaneous in the same temperature interval; the method is known as sinter- crystallization. By this method it is possible to produce a good sintered or porous glass material or a well-sintered or porous glass-ceramic material (in the case when during the heat processing results in significant crystallization). In the sinter-crystallization process the surfaces of the glass particles represent the nucleation centers, so it is not necessary to add a nucleus. The method of glass powder sintering is usually applied when surface mechanism of crystallization occurs or when there is



a need for making complex shapes of glass-ceramic materials. However, if the surface nucleation is fast, the growth of crystals will occur before full sintering. Therefore, in order to obtain a good sintered glass-ceramic product, it is important to know the crystallization characteristics and the sinterability of glass powders.

In this work the crystallization properties and sinterability of the lanthanum-strontium-borate glass powders will be presented. Crystallization behaviour of the glass was studied by the differentially thermal analysis (DTA), X-ray diffraction (XRD), transmission and scanning electron microscopy (TEM and SEM), while the sinterability of the glass powder was examined by the hot stage microscopy (HSM) and DTA [2,3].

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I-5

## **YAG:Ce,Pr YELLOW-EMITTING PHOSPHOR WITH ENHANCED RED EMISSION FOR WHITE LEDS**

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The most commonly used white light emitting diodes (LEDs) are the combination of blue-emitting chip and transparent yellow-emitting phosphor such as Y<sub>3</sub>Al<sub>5</sub>O<sub>12</sub>:Ce<sup>3+</sup> (YAG:Ce) which converts one part of blue light into yellow. The obtained yellow emission complements the transmitted blue light to yield the white light, usually called “cool white” due to red spectrum deficiency. In this study, the red spectrum component was introduced in the luminescence spectrum of YAG:Ce by doping with Pr. Fine YAG:Ce,Pr powders containing 0.3 mol% Ce and different amounts of Pr were synthesized by glycine nitrate combustion method starting from metal nitrates. Sintering of compacted powders was performed at 1600 °C for 10 h in air. The compacts were placed in a special setup consisting of two alumina crucibles filled with carbon powder in order to provide reducing atmosphere necessary to prevent oxidation of Ce<sup>3+</sup> and Pr<sup>3+</sup> ions and to avoid direct contact between samples and carbon powder. The purity of dense YAG samples obtained after sintering was confirmed by X-ray diffraction. The luminescent analysis under 450 nm excitation showed the typical Ce<sup>3+</sup> emission peak centered at ~ 540 nm overlapped with sharp red emission peak at about 610 nm. The red emission was ascribed to <sup>1</sup>D<sub>2</sub>-<sup>3</sup>H<sub>4</sub> transition in Pr. The energy transfer in YAG:Ce,Pr was studied with the help of excitation spectra.

I-6

## STRUCTURING OF HIGHLY POROUS MECHANICALLY STABLE SCAFFOLDS

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The bioinspired structuring of materials has been proven to be useful approach to tailor the materials' mechanical properties. Many different biomaterials have been used so far as a model. Among those biomaterials, cuttlebone stands out due to its high porosity (93 %) combined with an excellent mechanical stability – two properties that usually exclude each other. In this work we aimed at transferring cuttlebone's extraordinary structure-mechanic correlation to the multifunctional ceramic material  $V_2O_5$  by ice-templating.

Ice-templating of  $V_2O_5$  nanofibers results in an unique type of  $V_2O_5$  scaffolds, which exhibit an ultra high porosity (up to 99.8 %) coupled with mechanical stability allowing to bear more than 1000 times its own weight without failure. The obtained microstructure closely mimic that of cuttlebone lamellas arrangement. The lamellas are further connected by regularly arranged pillars, composed of nanofiber bundles, analogue to natural cuttlebone, but at much smaller dimensions. The cuttlebone-like microstructure of the  $V_2O_5$  nanofiber scaffolds was proved to be essential for achieving good mechanical stability by compressing cylindrical samples under uniaxial load. The use of flexible  $V_2O_5$  nanofibers unlocks further mechanical properties, going beyond bio-inspiration. Unlike other ceramic cellular solids, the here presented  $V_2O_5$  exhibit a pronounced mechanical flexibility, which allows to reversibly compress the scaffolds up to 3 % and leads to remarkable damping capacities ( $\tan\delta$  of up to 0.47).

The used multifunctional  $V_2O_5$  building blocks together with ultra-high porosity open a wide range of possible applications, including sensors, filters, catalysts and rechargeable batteries, which require a large surface area paired with mechanical stability.

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I-7

## **DEVELOPMENT OF ULTRA-HIGH TEMPERATURE CERAMICS BY FIELD ASSISTED SINTERING TECHNOLOGY**

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A new type of ceramic material for extreme applications was developed by introducing the Lu<sub>2</sub>O<sub>3</sub> sintering additive (2, 5, and 10 wt.%) into the well-known and commonly used ZrB<sub>2</sub> - 25 vol.% SiC material system to improve the high temperature properties of ZrB<sub>2</sub>-SiC ceramics. Other two rare-earth oxides (Yb<sub>2</sub>O<sub>3</sub> and Eu<sub>2</sub>O<sub>3</sub>) with different quantities (2, 5, and 10 wt.%) were separately introduced into the mixture of ZrB<sub>2</sub> and SiC using the most promising ball milling process. The sintering process was optimised and all the materials achieved a relative density above 98% when sintered using the Field Assisted Sintering Technology at a temperature range of 1950–2050 °C, pressure of 70–90 MPa, with a dwell time of 7 min, and Ar atmosphere. All the investigated ZrB<sub>2</sub> - 25 vol.% SiC-RE<sub>2</sub>O<sub>3</sub> materials exhibited superior room temperature mechanical properties to the reference ZrB<sub>2</sub> -25 vol.% SiC system. The ablation resistance of the materials was investigated using an oxyacetylene torch up to ~2650 °C, in order to determine the ultra-high temperature properties of the materials. The effect of different rare earth additives and different quantities on the ablation resistance of the materials was thoroughly investigated.

*Acknowledgment:* This work was supported by the Slovak Research and Development Agency under the contract no. APVV-SK-SRB-18-0022 and APVV-17-0328. The support of the Joint Mobility Project within Czech-Slovak scheme for the period 2018–2020 under the ASCR-SAS agreement is also acknowledged.

I-8

## ALUMINA FORMING MAX PHASES: CURRENT STATUS AND FUTURE PERSPECTIVES

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MAX phases are a family of 70+ ternary carbides and nitrides, and even larger number of their solid solutions, that share common unique naonolayered structure and chemical formula  $M_{n+1}AX_n$ , where  $n = 1, 2$  or  $3$ ,  $M$  is and early transition metal,  $A$  is an A-group element (mostly IIIA and IVA) and  $X$  is either C or N [1]. The main reason for growing interest in MAX phases lies in their unusual, and sometimes unique combination of properties. In general, MAX phases are elastically stiff, good thermal and electrical conductors, resistant to chemical attack, and have relatively low thermal expansion coefficients, but also relatively soft and most readily machinable, thermal shock resistant and damage tolerant [2]. Some of them are fatigue, creep, and oxidation resistant. Most importantly for their applications at high temperature, some of them - most notably  $Ti_2AlC$  and  $Cr_2AlC$  - shows exceptional oxidation resistance due to formation of the protective, self-healing and adherent alumina protective oxide scale.

In this lecture, our current understanding of what makes some of the MAX phases exceptionally oxidation resistant will be discussed in more details. Oxidation mechanisms and kinetics observed in different alumina forming MAX phases are reviewed. It has been well established by now that both  $Ti_2AlC$  and  $Cr_2AlC$  show cubic oxidation kinetics in 1000–1400 °C temperature range [3–5]. However, while  $Ti_2AlC$  forms only pure alumina oxide after short trainset regime,  $Cr_2AlC$  forms top alumina layer with  $Cr_7C_3$  layer beneath. We have shown recently that morphology of the oxide layer depends on the amount and type of impurities present in MAX phase.

As Al diffuses from MAX phase towards the oxide scale, MAX phase substrate becomes depleted on Al, which finally results in decomposition of the alumina forming MAX phase and breakaway oxidation. Herein we report for the first time results of systematic study of breakaway oxidation in MAX phases using wage shaped samples. Oxidation of wage shaped samples suggest that  $Ti_2AlC$  decomposes after losing around 5% of Al. Once that happened, oxide layer is not protective anymore as it contains substantial amount of titanium-oxide.

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I-9

## **MAX MATERIALS AND COATINGS STABLE IN OXIDIZING AND HYDROGEN ATMOSPHERES AT HIGH TEMPERATURES**

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The paper is considered Ti,Nb-Al-C MAX phases-based materials (of 211 and 312 structural types) synthesized by hot pressing (at 15–30 MPa) and coatings (of 311 structural type) deposited by the vacuum-arc method with a planetary rotation using dense MAX-phases-based targets (synthesized by hot pressing). The synthesised materials and deposited coating occurred to be stable in oxidizing (at least for 1000 h) and hydrogen (at least for 40 h) atmospheres at 600 °C. The electrical conductivity of the surface of Ti<sub>3</sub>AlC<sub>2</sub>-based coating after heating for 1000 h at 600 °C in air stayed practically unchanged and was  $1.2 \times 10^6 \text{ S} \cdot \text{m}^{-1}$  (estimated by a four-probe method). Ti<sub>2</sub>AlC-, Ti<sub>3</sub>AlC<sub>2</sub>- and (Ti,Nb)<sub>3</sub>AlC<sub>2</sub>-based materials are more stable in air than Cr-containing Crofer steels and about twice lighter ( $\rho \approx 4.27 \text{ g/cm}^3$ ). The most resistant in air at 600 °C among the studied bulk materials turned out to be Ti<sub>2</sub>AlC-based and somewhat less stable occurred to be (Ti,Nb)<sub>3</sub>AlC<sub>2</sub>- and Ti<sub>3</sub>AlC<sub>2</sub>-based. The Auger study confirmed the presence of some oxygen in the structure of Ti<sub>2</sub>AlC, what can be the explanation of their high stability against oxidation. The addition of Nb increased stability of Ti<sub>3</sub>AlC<sub>2</sub> in oxidizing atmosphere and leads to about four time's thinner oxide film. The stability in air at 600 °C of Ti<sub>3</sub>AlC<sub>2</sub>-based material was increased by preliminarily oxidation at 1200 °C. The bending strength of Ti<sub>3</sub>AlC<sub>2</sub>-based material in air at 20 °C was 535 MPa, after been keeping at 600 °C in air and hydrogen it decreased to 490 and 500 MPa, respectively. For (Ti,Nb)<sub>3</sub>AlC<sub>2</sub>-based materials the bending strength at 20 °C in air was 480 MPa and increased for 10% after heating at 600 °C both in air and in hydrogen. The high temperature X-rays showed that bulk Ti<sub>2</sub>AlC was oxidized more intensive than Ti<sub>3</sub>AlC<sub>2</sub> at higher temperatures (Ti<sub>2</sub>AlC was stable up to 700–750 °C and Ti<sub>3</sub>AlC<sub>2</sub> - up to 1050–1100 °C). The most stable at thermal cycling up to 1200 °C was a high-density material based on the MAX phase Ti<sub>3</sub>AlC<sub>2</sub>, obtained by two-stage technology (synthesis in vacuum with subsequent compression by hot pressing at 30 MPa).

I-10

## TOPOTAXIAL PHASE TRANSFORMATIONS AND TWINNING OF RUTILE

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Topotaxial phase transformations (TPTs) are processes controlled by solid-state diffusion leading to oriented exsolutions of secondary phases inside the host crystal. They are commonly characterized by high spatial coherency between the parent phase and the product phases, whereby the host sublattice is reconstructed to adopt a new structure with the lowest possible cost of energy. Product/host orientation relationships follow the simple energy principle – higher is the coherency, lower is the energy of transformation, and vice-versa. The resulting orientation relationship bears information on p-T conditions as well as reaction rate, while chemical composition of the product holds the evidence on what triggered the particular transformation. While departure from chemistry is generally a trigger of transformation, a dopant concentration (e.g.  $f\text{O}_2$ ) at given p-T conditions defines the reaction rate and involved diffusion processes.

In this talk we will see few examples of crystallographically different oriented intergrowths of rutile ( $\text{TiO}_2$ ) dictated by TPTs from structurally related Fe-Ti oxides and oxyhydroxides. The product of these reactions are reticulated networks of rutile, interconnected through complex crystallographic laws. Due to tetragonal deviation of rutile from the ideal *hcp* structure the angle between [001] and [101] of O-sublattice is  $57.2^\circ$ . This has a decisive effect on modes of rutile exsolution from structurally related minerals [1]. During exsolution from the precursors with ideal *hcp* oxygen sublattice (e.g. ilmenite), the c-axes of rutile domain may be parallel to three equivalent  $\langle 210 \rangle$  directions of the precursor and they intersect at  $60^\circ$  [2]. However, when [101] of rutile is aligned parallel to  $\langle 210 \rangle$  of the host, rutile's c-axis is deflected for  $2.78^\circ$  due to tetragonality, resulting in more complex rutile intergrowths, among which the most common are rutile twins on (101) and (301) planes [3,4]. The studies of TPTs at the nanometer scale are supported by complementary electron microscopy and spectroscopy methods.

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I-11

## **MATERIALS WITH EXCITED QUANTUM COHERENCE: FROM PLASMONICALLY INDUCED TRANSPARENCY TO QUANTUM CORRELATION**

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Spectroscopy of materials can be enhanced by the quantum coherent effects [1,2]. Quantum coherent effects are demonstrated to have an all-optical control, on ultrafast time scales, over the photonic topological transition [3]. Localized plasmon interaction in quantum confined structures strongly modify the optical and electronic properties with potential for manipulating light on the nanoscale [4]. Transient pump-probe spectroscopy demonstrates that the coherent absorption in quantum dots is modified by phonon-assisted plasmon induced transparency. A theoretical model has been developed to quantitatively demonstrate that the dark states can be still formed at ultrashort time scale corresponding to the dephasing time of the carriers in the quantum dots. The demonstrated results are important for developing new sensors based on high nonlinearities and their applications to optoelectronic devices. Another approach to demonstrate quantum coherent and cooperative effects is to study the Bi-exponential decay of dye fluorescence near the surface of plasmonic metamaterials and core-shell nanoparticles that has been shown to be an intrinsic property of the coupled system [5]. Our theory shows that the relaxation leads to the population of the sub-radiant states by dephasing the super-radiant Dicke states giving rise to the bi-exponential decay in agreement with the experiments. We use a set of metamaterial samples consisting of gratings of paired silver nanostrips coated with Rh800 dye molecules, having resonances in the same spectral range. We have demonstrated the spectroscopy of nanomaterials and metamaterials, where the quantum coherent effects are able to have an all-optical control, on ultrafast time scales, over the photonic topological transition, for applications as varied as quantum sensing, quantum information processing, and quantum simulations using metamaterials.

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I-12

## **NANOSIZED SEMICONDUCTING MATERIALS - THEIR PROPERTIES AND APPLICATIONS – THEORETICAL APPROACH**

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Materials in nanoscale are still increasingly used in many applications. It is due to their unique properties, completely different from the native materials, arising from their size limitation. Moreover, a doping, surface modification and shape tailoring may change the physical properties of nanocrystals. Semiconducting nanoparticles are popularly used in photovoltaic and photocatalytic applications, where the most known are titanium oxide, zinc oxide and bismuth vanadate based materials. Their electronic and optical features are modulated in large extents when metal ions and sensitizing dye molecules are used. The reactive surface area with its defects and vacancies acting on the charge transfer peculiarities enhance the efficiency of solar cells, energy storage and photocatalysis. Computer simulations and quantum chemical calculations can explain the nature of charge transfer phenomena occurring in the mentioned materials acting on their electronic properties.

This work presents the theoretical approach to predict the electronic properties of selected semiconducting nanostructures. The influence of vacancies and surface anchored molecules on their electronic properties will be shown [1]. In this case, the original cluster approach methodology was developed [2]. The electronic properties of the hybrid systems were calculated by quantum-chemical methods applying DFT and semi-empirical approach. Was proved that nanostructures exhibit a patchwork properties of the bulk material, amorphous structures and atoms located at the surface of the investigated cluster [3]. The influence of dopants on electronic properties of the nanoparticles was also discussed. It was proved that the nature of vacancies located close to the dopants is crucial in the design of advanced materials.

*Acknowledgment:* This work was partly financially supported by National Science Centre, Poland, within the project No. 2017/25/B/ST8/01864.

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I-13

## **THEORETICAL INVESTIGATION OF MAGNETIC AND MULTIFERROIC PROPERTIES**

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Over the past decade, the research activities on magnetic and multiferroic materials have been totally renewed both from the experimental and theoretical sides. Here we will show how Density Functional Theory (DFT) calculations combined to Monte-Carlo simulations can be used to support experiments and predict new properties. A particular focus will be done on the way we estimate magnetic exchange parameters, magnetic anisotropy and temperature-pressure effects. Copper oxides and oxyhalides will be considered to illustrate the impact of chemical and physical pressures on magnetic and multiferroic properties.

I-14

## **PLASMON ENHANCED VISIBLE LIGHT PHOTOCATALYTIC ACTIVITY IN POLYMER-DERIVED TiN/Si-O-C-N NANOCOMPOSITES**

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The collective resonant oscillation of conduction electrons upon the illumination of incident light in metallic nanocrystals is generally known as localized surface plasmon resonance (LSPR) [1]. Extensive studies have been carried out in the field of photocatalytic enhancement exploiting LSPR phenomenon. The intensity and wavelength of LSPR hugely depends on the size and morphology of the nanostructures [2,3]. The photocatalytic reaction based on plasmonic mechanism involves either a combination of a metallic nanoparticle and a semiconductor or pure metal plasmonic catalysts. The former involves a reaction happening between a semiconductor surface and a plasmonic nanoparticle thereby aiding the visible light absorption. The latter one involves transfer of ‘hot’ electrons to the lowest

unoccupied molecular orbital (LUMO) of adsorbate molecules, thus weakening the chemical bond and increasing the reaction rate. Noble metals such as Au, Ag and Pt harness visible light in the solar spectrum owing to the LPSR and exemplify an essential class of plasmonic structures [4,5]. The plasmonic structures have wide range of applications such as sensing, biophotonics, photovoltaics, waveguiding and photocatalysis [6,7]. However, the high cost and thermal stability issues in these nanostructured components limit their practical applications and hence alternative materials should be explored.

Herein, we provide a detailed insight into the precursor chemistry, precursor-to-material transformation and characterization of nanocomposites made of a TiN nanophase and a Si-O-C-N ceramic. The polymer-derived ceramics (PDCs) route applied to synthesize these nanocomposites resulted in the formation of nanocrystals less than 4 nm in size and the calculated lattice parameter value for the nanocrystals ( $a = 0.4239$  nm) matched the theoretical value of TiN ( $a = 0.4241$  nm). The Si-O-C-N ceramic served as a platform for anchoring TiN nanocrystals. As a proof of concept, we have attempted to exploit the plasmonic properties of nanocomposites to achieve photocatalytic degradation of organic dyes. The absorption spectra clearly showed plasmonic resonance in the visible region with peak positioned around 670 nm according to the presence of TiN nanocrystals which resulted in the enhancement of dye degradation.

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I-15

## MICROSTRUCTURE CONTROL IN MULTIFERROIC COMPOSITES

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Magnetoelectric multiferroics are a special class of multifunctional materials with coupled ferromagnetic and ferroelectric orders. They are of great interest because they not only show the characteristic of the single ferroic orders where the electric field E, and the magnetic field H, control the electric polarization P and magnetization M, respectively, but also because interactions between them lead to additional functionalities. A wide range of applications has been proposed and demonstrated, due to their tunability, electronic and magnetic properties [1]. The composites are produced as bulk [2] and thin or thick [3] film structures where the connectivity of the phases plays a critical role; the 3-0 -type particulate structure and the 2-2 type laminate structure are the most promising in terms of maximization of the interfacial coupling between the magnetic and the ferroelectric phase.

The powder synthesis approach and the careful design of any processing step (ex. milling after calcination [4], control of the stoichiometry by preventing the loss of volatile species [2]) let to control the microstructure in cobalt ferrite (CFO) composites with PZT or BNBT. Composites with different molar ratio of the two phases were prepared by solid state reaction [5] or by sol-gel synthesis, including core-shell-type nanostructures [6] and thin films [7] of composition BNT-BT<sub>0.08</sub>/CFO. The densification of the materials is a critical step to achieve the ideal microstructure with nanosized CF grains well dispersed in a fully dense matrix of BNBT or PZT micrometric grains. Fully dense materials with nanosized CFO grains dispersed in the ferroelectric matrix were successfully produced and characterized.

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I-16

## **RADIOLABELLED NANOMATERIALS DESIGNED FOR APPLICATION IN MEDICINE**

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Iron oxide magnetic nanoparticles (IONPs) have been subjected to a variety of biomedical applications due to their remarkable nanoscale physicochemical properties. Their small size, high surface to volume ratio and size-dependent magnetic properties make them ideal candidates for clinical applications, including magnetic resonance imaging, in which they serve as T2-contrast enhancement agents [1], hyperthermia treatment of cancer [2], cell separation, tissue repair [3], and magnetic force guided drug delivery. Magnetite (Fe<sub>3</sub>O<sub>4</sub>) and its oxidized form maghemite (Fe<sub>2</sub>O<sub>3</sub>) are the most common IONPs, which compose the core in a typical core-shell nanoparticle structure. Thanks to the ease of surface functionalization, IONPs are provided with colloidal stability via steric and electrostatic interactions and high loading capacity via functional (i.e., hydroxyl, carboxyl, amino, and thiol) groups, in order to be bound with many active targeting molecules (such as antibodies, aptamers, and peptides), drugs, and detection elements (i.e., radionuclides for molecular imaging, fluorescent molecules) according to demand in biomedical applications. Radiolabelled nanoparticles represent a new class of agent with great potential for nuclear medicine applications.

In the present work IONPs based on the magnetite core coated with different compounds (albumin, citrate, PEG, DPD) were synthesized in order to compare their efficiency as radioactive vectors. Coatings increased colloidal stability of IONPs and allowed binding of radionuclides for the functional groups on their surface. The IONPs were characterized based on their structure, morphology, size, surface charge, and magnetic properties. Several radionuclides interesting for the potential use in localized hyperthermia-radionuclide therapy as well as for the application in dual-modality PET (SPECT)/MRI were investigated: <sup>90</sup>Y, <sup>177</sup>Lu, <sup>99m</sup>Tc and <sup>68</sup>Ga. Radiolabelling conditions such as pH, concentrations of IONPs and reaction time were varied to obtain maximum radiolabelling yield.

IONPs showed favorable phase purity, physicochemical and magnetic characteristics for *in vivo* use. Labelling yield >97%, high *in vitro* and *in vivo* stability and satisfactory *in vivo* behaviour of radiolabelled IONPs, create opportunities for their use in combined radio-hyperthermia cancer treatment and dual-modality imaging.

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I-17

### 3D PRINTING OF MULTIMATERIAL GLASS AND CERAMIC OPTICS

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The ability to 3D print transparent glass and ceramics holds the potential to impact applications ranging from microfluidics to optics. Multimaterial printing offers incorporating diverse functionalities by spatial control of material composition. The addition of dopants to the base glass or ceramic material imparts modifications in their optical or mechanical properties. In this regard, multimaterial additive manufacturing (AM) of transparent glass and ceramics could enable the production of advanced optics with tailored properties. We have developed an approach to 3D print multimaterial glasses and ceramics for optical applications using direct ink writing (DIW). The multimaterial construct is printed from particle-based slurries (doped and undoped). The green body is printed with a prescribed gradient or discrete distribution of dopant concentration, and then thermally treated to form a dense, transparent product with spatial change in optical properties. We demonstrate successful fabrication of gradient index (GRIN) silica-titania glass lenses, as well as core-cladding Nd:YAG (Y<sub>3</sub>Al<sub>5</sub>O<sub>12</sub>) laser gain media. This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 within the LDRD program 16-SI-003. LLNL-ABS-772084.

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I-18

## **PREPARATION AND MECHANICAL PROPERTIES OF POROUS ZIRCONIA/CALCIUM PHOSPHATES CERAMIC COMPOSITES**

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Stabilized zirconia ceramic with good mechanical properties, is widely applied for orthopedic and dental restoration. Zirconia is a biocompatible but bio-inert ceramic material, meaning it poorly or not at all interacts with the surrounding tissue and cannot connect with hard tissues. Stabilizing compounds such as yttria, magnesia, ceria, and alumina are commonly used to stabilize the metastable tetragonal phase in a zirconia, thus enabling transformation toughening. On the other hand, calcium phosphate (CaP) based biomaterials are often used as coatings for bio-inert metal and polymer implant materials.

In this study mechanical stability of porous ZrO<sub>2</sub> ceramics biomimetically coated with calcium deficient hydroxyapatite (CaDHA) as bioactive materials, was investigated. With the aim to prepare bioactive materials for bone implants, we investigated growth and stability of CaDHA coating on porous yttria stabilised tetragonal zirconia ZrO<sub>2</sub> obtained by sol-gel process and sintering at 1400 °C. The coating with was performed by immersion of ceramics in a calcifying solution. In order to test their suitability as a material for possible bone implants mechanical properties of these composite bioactive ceramics was tested by ball to ball compression test, indentation hardness test and by scratch test.

It was observed that the coverage of the zirconia ceramic surface by CaDHA depends on the washing procedure applied before the immersion. Vickers hardness, tensile strength and Weibull modulus of ZrO<sub>2</sub>-CaP biomaterials matched or exceeded those of bone. The tensile strength was somewhat improved for the coated as compared with the uncoated ceramic due to CaDHA filling the surface defects from which cracks can initiate. The scratch test indicated good adhesion of the CaDHA coating on the surface of zirconia. These results indicate the potential usage of proposed bioceramic for bone implants.

*Acknowledgment:* Croatian-Austrian bilateral project (OeAD WTZ project HR 04/2014), HRZZ project IP-2018-01-1493, Centre of Excellence for Advanced Materials and Sensing Devices, Ruđer Bošković Institute, Zagreb, Croatia, COST Action MP 1301.

I-19

## **RELAXOR FERROELECTRIC CERAMICS FOR ELECTROCALORIC COOLING: PROCESSING CHALLENGES AND POSSIBLE APPLICATIONS**

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Increasing needs of society for electricity, heating, or cooling have become a global priority, thus efficient ways of energy production, conversion, storage, and consumption are needed. A contribution to solutions to such problems may be implementation of nonlinear dielectrics (ferroelectrics, relaxor ferroelectrics, antiferroelectrics) in cooling by exploiting the electrocaloric (EC) effect. The latter is defined as a reversible temperature change in a material upon application of an external electric field at adiabatic conditions. Materials exhibiting a large EC effect over a temperature range of a few 10 K close to room temperature include lead-based complex perovskites, such as  $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3\text{-PbTiO}_3$  [1,2] solid solution or their lead-free counterparts, such as  $(1-x)(\text{K}_{1/2}\text{Na}_{1/2})\text{NbO}_3\text{-xSrTiO}_3$  [3] with compositions exhibiting a pronounced relaxor character. Typical EC temperature changes reported for bulk ceramics are a few K at electric fields of about 100 kV/cm, which is close to the dielectric breakdown strength of respective materials.

Multilayer ceramic elements have been shown to sustain higher electric fields than bulk ceramics which can be also related to the lower thickness of individual layers, and consequently they also need lower applied voltages, which is suitable for applications. In the contribution we report a comprehensive EC study of  $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$  (PMN) [4] and  $0.9\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3\text{-}0.1\text{PbTiO}_3$  (PMN-10PT) [5] ceramics in forms of bulk and multilayer elements for potential use in cooling devices. We discuss the importance of synthesis and processing in obtaining phase-pure perovskite materials that exhibit a fatigue-less electrocaloric effect even upon extended unipolar electric field cycling.

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I-20

## EXPERIMENTAL EVIDENCE OF ELECTRO-MECHANICAL COUPLING IN CUBIC YSZ

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Cubic ZrO<sub>2</sub> doped with 8 mol% Y<sub>2</sub>O<sub>3</sub> (8YSZ) has been one of the well-known solid state ionics for applications in solid oxide fuel cells (SOFCs) and oxygen sensors. Oxygen vacancies formed as a result of doping with Y<sub>2</sub>O<sub>3</sub> can freely move at high temperatures (above 600 °C) leading to the high ionic conductivity of the material. However, at low temperatures (below 600 °C), oxygen vacancies are trapped by immobile opposite charged cations even in dilute solutions in cation-oxygen vacancy clusters - a simplest one of which is  $(Y'_{Zr}V''_O)^{\bullet}$ . Those clusters are electric and elastic dipoles and when the material is heated at temperatures above 100 °C, oxygen vacancy can hop to another position around the dopant cation to change the dipole orientation under applied electric field or mechanical stress. We have shown that starting from that temperature it is possible to record electric field-polarization hysteresis loops due to reorientation of cation-oxygen vacancy dipoles. Since the crystal lattice deformation depends on dipoles orientation and vice versa it is possible to change hysteresis shape and size by application of mechanical stress in direction parallel to electric field. At temperature above 500 °C diffusion processes and thermal vibrations are so pronounced that interactions between cation and oxygen vacancies are too weak to hold them together, i.e. dipoles dissociate and 8YSZ becomes conductive. The existence of dipoles that could be reoriented in temperature interval from 100 to 500 °C has been also proved in this study by piezo measurements. Sinusoidal mechanical stress induced sinusoidal electric response and piezoelectric parameter  $g_{33}$  was calculated. Parameter  $g_{33}$  is both temperature and frequency dependent and increases with increase in temperature and frequency. At temperature of 330 °C and frequency of 10 Hz value of  $g_{33}$  of the 8YSZ was  $5.08 \cdot 10^{-8}$  Vm/N. Unlike to ferroelectric materials in which piezoelectric coupling is related to domain switching, the observed effect in 8YSZ is related to the reorientation of electric dipoles under applied stress and electric field.



I-21

## ENGINEERING OF DEFECTS AND THERMOELECTRIC PROPERTIES OF ZnO CERAMICS

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ZnO is a promising n-type thermoelectric oxide material with a reported  $zT$  value of 0.45–0.65 at 1000 °C. As well as being nontoxic, inexpensive and stable in air to high temperatures, it has a high  $S$  of about  $-400 \mu\text{V/K}$  and excellent charge-carrier transport properties that are easily tunable via doping. Unfortunately, it also has a large lattice thermal conductivity due to its simple Wurtzite structure. The simultaneous optimization of compositional, structural and microstructural features, which would result in a high  $\sigma$  while preserving a high  $S$ , and a drastically reduced  $\kappa$  remains a great challenge, despite many efforts.

Doping the ZnO with selected elements and in combination with processing conditions resulted in markedly enhanced solid solubility of donor dopants in the ZnO grains and reduced resistivity of the grain boundaries; hence the ZnO ceramics had extremely high electrical conductivity and among the highest power factors reported for the ZnO in the literature. Accordingly, engineering of point defects in the ZnO grains and at the grain boundaries will be discussed. Furthermore, doping with oxides of In or Ga causes nanostructuring in the ZnO wurtzite structure with the formation of multiple planar defects. In the case of  $\text{In}_2\text{O}_3$ -doping the highest  $zT$  values were reported for the homologous phase  $\text{Zn}_5\text{In}_2\text{O}_8$  with a high density of planar defects. However, our results showed that these defects are formed in some ZnO grains already for additions of In and Ga much below 1 at.%, causing increase of electrical conductivity and a decrease of thermal conductivity, so indicating a broad window for further optimizations.

I-22

## DIELECTRIC AND ANELASTIC SPECTROSCOPY: A POWERFUL COMBINED TOOL FOR CHARACTERIZING MULTIFUNCTIONAL CERAMICS

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Dielectric and anelastic spectroscopies are complementary techniques and their combination allows valuable information to be obtained in the field of multifunctional materials. Whereas the dielectric spectroscopy measures the dielectric susceptibility  $\chi(\omega, T)$  and it is sensitive to fluctuations of electric dipoles, the anelastic spectroscopy measures the elastic compliance or elastic susceptibility  $s(\omega, T)$  and it is sensitive to fluctuations of elastic dipoles. Both susceptibilities are complex, their imaginary part being due to the delayed response of the mobile defects coupled to the electric field/stress. The great advantage of using a combination of both techniques is that the anelastic measurements are insensitive to free charges, therefore it is possible to measure the dynamics of ions also in the presence of free charges.

Two main types of investigations have been pursued by the combination of these techniques: the study of structural phase transitions and the study of microscopic mechanisms associated with the presence of defects, both important for the knowledge and development of multifunctional materials. We have applied this approach for different functional materials with perovskite framework: multiferroic, ferroelectric and relaxor ferroelectric ceramics, and organic-inorganic perovskite photovoltaics. Thanks to the combination of the two spectroscopies, it has been possible to probe more accurately the structural transitions involving the antiferrodisortive tilt modes of the octahedra in PZT [1] and NBT-BT [2]. It was also possible to evidence incipient phase separation in lead titanate-based multiferroics [3]. Moreover, since the elastic response is insensitive to free charges, it has been used to probe the piezoelectric response even in unpoled ceramics [4] and for the study of coexisting ferroelectric and metallic states [5]. The combination of the two techniques allowed also new features to be revealed on the reorientation dynamics of the organic molecules in MAPbI<sub>3</sub> photovoltaic organic-inorganic perovskites and the hindrance of their ferroelectric order by coupling with the tilt modes [6].

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I-23

## **VARIABLE RANGE HOPPING MECHANISM OF CARRIER TRANSPORT IN BiFeO<sub>3</sub> NANO-PARTICLES REVEALED VIA RAMAN SCATTERING TECHNIQUE**

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Single-phase multiferroic BiFeO<sub>3</sub> compound has recently captivated much attention because of its desirably high ferroelectric Curie temperature of ~1100 K and antiferromagnetic Néel temperature  $T_N$  of ~640 K, which both slightly decrease with decreasing crystallite size. As such, BiFeO<sub>3</sub> at nanoscale proves to be promising for prospective applications in memory smart devices, satellite communications, novel sensing technologies, and spintronics. In order to meet these industrial requirements, the electric resistance of BiFeO<sub>3</sub> nanopowders must far exceed low insulation electric transport values, of which mechanism is hard to capture using contact probes. As highly informative experimental tool, Raman spectroscopy demonstrates ability to assess the nature and dynamics of charge carriers in conductive systems in a contactless indirect manner. In the present study we have analyzed broad electronic Raman scattering response of BiFeO<sub>3</sub> nanoparticles as a function of temperature (80–723 K) from which the carrier scattering rate can be estimated [1]. Two different 3D phonon-assisted Variable Range Hopping (VRH) electron transport mechanisms have been detected. VRH model due to Mott [2] is accompanied with the high-temperature paramagnetic phase (above  $T_N$ ), whereas the VRH mechanism based on Efros & Shklovskii model [3] has been revealed in the strongly correlated low-temperature phase (below  $T_N$ ). Our preliminary estimation of the electronic density of states above  $T_N$  exceeds number of  $10^{19}$  electron states per (eV cm<sup>3</sup>), which is in agreement with the finding by Ruby & Inbanathan [4] obtained directly from DC electrical resistivity measurements in doped BiFeO<sub>3</sub> thin films. In both cases the electron localization length has been found to closely match the average nanoparticle size of few tens of nanometers. This finding indicates that the system is disordered enough to localize the charge-carrier states within the nanoparticles.

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I-24

## **ELECTRON SPIN RESONANCE STUDIES OF NATURAL KAOLINITES: A BRIEF REVIEW**

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Kaolinite is extensively used when pure as cheap, general-purpose filler and coating material in ceramics. The commercial value of natural kaolinite is greatly affected by the presence and content of trace metals impurities, which can effect, for example, the whiteness of manufactured products. Many of these impurities are transition metal ions ( $\text{Fe}^{3+}$ ,  $\text{VO}^{2+}$ ,  $\text{Cr}^{3+}$  and  $\text{Mn}^{2+}$ ) and they are electron spin resonance (ESR) active. For this reason, ESR spectrometry has been used frequently to study natural kaolinites containing these ions.

As early as 1961, Boesman and Schoemaker published a short paper titled: Resonance paramagnetic de l'ion  $\text{Fe}^{3+}$  dans la kaolinite [1]. Since then, numerous ESR studies have been carried out on natural kaolinites from weathering, sedimentary and hydrothermal environments. The work of Laboratory for Geochemistry, Cosmochemistry and Astrochemistry (LGCA in this research field was recognized by international scientific community. The first paper dealing with the ESR of natural kaolinites was published in 1984 [2]. This work was focused on sedimentary (well-ordered) kaolinite (KGa-1, Fig. 1) from Georgia, USA. The researchers of LGCA carry out many detailed studies of numerous sedimentary (poor-ordered) kaolinites from France and Serbia, well-ordered sedimentary kaolinite from Georgia (KGa-1 and KGa-2) and England, and well-ordered hydrothermal kaolinites from Mexico and Canada, and hydrothermal dickite from Poland. This presentation is focused on these previous studies of natural kaolinites (and related clay minerals) of LGCA (Table 1) in combination with the similar works of other researcher groups worldwide.

LGCA combined various geochemical and spectroscopic approaches to study kaolinites presented in Table 1. The key aims of these studies was to identified by ESR  $\text{Fe}^{3+}$ ,  $\text{VO}^{2+}$  and  $\text{Cr}^{3+}$  ions and to define the nature of their immediate chemical environments in the clay structure. These experimental data were then employed: (a) to suggest possible origin of these metal ions in the kaolinites studied, (b) to estimate their physicochemical conditions of their formation and (c) to study their thermal stability. It is worth to note here that LGCA developed a very original method of quantification of  $\text{VO}^{2+}$  ions in kaolinites.

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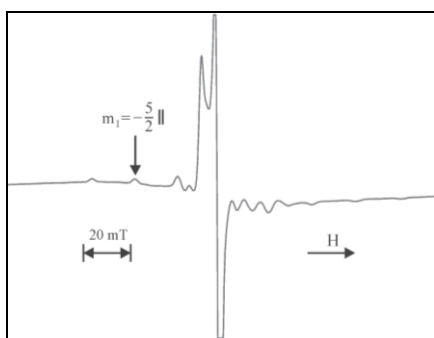


Figure 1. ESR spectrum of the KGa-1 kaolinite

Table 1. Location, type, and origin of the selected kaolinites and kaolinite-rich sedimentary samples

Sample name	Location	Type	Origin
KGa-1	Georgia (USA)	Well-ordered kaolinite	Sedimentary
BCH5	Charentes (France)	Poorly-ordered kaolinite	"
BCH6	"	"	"
CHA2	"	"	"
LAP1	"	"	"
SGN2	"	"	"
SGN3	"	"	"
FBT2	"	"	"
FBT 4	"	"	"
FBT 2A-02	"	"	"
FBT 2A-03	"	"	"
FBT 3A-01	"	"	"
FBT 3A-02	"	"	"
FBT 3A-03	"	"	"
Provins	Paris Basin (France)	"	"
Arandelovac	(Serbia)	"	"
Kolubara	"	"	"
GB1	Cornwall (England)	Well-ordered kaolinite	"
CNS	New Mexico (USA)	Shale	"
SVS	"	"	"
Zvonce	Zvonce (Serbia)	"	"
Cigar Lake	Saskatchewan (Canada)	"	Hydrothermal
Nopal	Chihuahua (Mexico)	Well-ordered kaolinite	"
Nowa Ruda	Silesia (Poland)	Well-ordered dickite	"

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## **TRADITIONAL CERAMICS: PAST, PRESENT AND FUTURE**

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In this paper review of the traditional ceramics will be given. Different types of ceramics will be discussed, in correlation with historical time and use, as well as the present time and future perspectives of traditional ceramics. Processing of the traditional ceramics, as well as differences in processing during time will be also discussed. Past of the traditional ceramic will be focused on pottery, glass and construction and optic materials. Present time will include traditional engineering ceramic. Traditional ceramics in future will be related to the possible application and synthesis of modern ceramic materials.

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I-26

## ECO-CERAMICS FOR BLAST MITIGATION

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The improvements of physical, chemical and thermomechanical properties of composite materials have been a major research interest in the last few decades. The fly ash resulting from burning coal is one of the most important wastes are produced in the world, including Romania and its historical dumps or currently generated has become a real challenge for researchers. Generating massive ash coal firing thermal power plant involving environmental and economic issues, as far as storage of such waste has recently become stricter because of environmental regulations and high costs related to waste disposal. Physical and chemical properties of ash obviously depend on the type of coal used and combustion conditions. The coal ash contains valuable oxides, such as: SiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, CaO, Fe<sub>2</sub>O<sub>3</sub> and other oxides; and a variable composition, density, texture, porosity and water absorption capacity. It was investigated a new possibility to use abundant ash waste from coal burning through a rapid thermal treatment of ceramic composite bodies [1]. The chemical properties of ash from burning coal samples show appropriate characteristics, being comparable with those of ceramic materials commonly used in the ceramics industry. Internationally, research is still underway in order to determine effective methods to dissipate explosive energy and to contain explosive overpressure using blast-mitigating materials. This paper introduces the polymeric matrix impregnated with suspensions of fly and bottom ash and glass cullets for lightweight cellular structure development devoted mainly for blast protection and mitigation of their effects. The results show that the development of such lightweight ceramic can be effective in appropriate heat treatment conditions in electrical furnace as well as in microwave field at 2.45 GHz. The ceramic properties recommend them as lightweight aggregate in construction, also. In the medium term, the use of lightweight aggregates in the construction industry is expected to grow taking into account technical and economic advantages: raw materials at low cost, rapid processing and environmental protection.

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I-27

## **SELF-SUPPORTING ZEOLITES BY GEOPOLYMER GEL CONVERSION: EVALUATION FOR WATER SOFTENING APPLICATIONS**

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In several industrial applications, such as water softening, supporting or shaping powdery zeolites is a technological urgency. In fact, structuring a porous powder, like a zeolite, allows attaining better performances in terms of mass transfer, chemical and mechanical stability. Zeolites are employed to a large extent as water softeners. It is well known that zeolites Na-A and Na-X can exchange their sodium ions with “hard water ions”, such as calcium and magnesium. It has been also demonstrated that a synergistic effect can be reached using a mixture of them. Due to their similarities, it is possible to promote zeolite crystallization inside a geopolymeric matrix by tuning pH, temperature and time of the geopolymerization reaction [1,2].

In the present work, a self-supporting zeolitic filter was synthesized by a one-step procedure, realizing simultaneously geopolymerization and crystallization under mild operating conditions (40 °C), without further treatments. The geopolymer gel precursors were prepared by mixing metakaolin, silicon powder and sodium hydroxide solution. The geopolymer conversion also generates a hierarchical porosity characterized by mesoporosity (typical of the geopolymer matrix) and microporosity (characteristic of the zeolitic phases), while the addition of the silicon powder is intended to widen the porosity of the sample also to the macro range: under alkaline conditions, silicon reacts developing hydrogen, which promotes an *in situ* inorganic foaming [3]. The specimens obtained after 3 days of curing or more showed the presence of two distinct phases, identified as zeolites Na-A [LTA] and 13X [FAU], the relative quantity of each phase being strictly related to the experimental conditions used. The nucleation and growth of both phases were completed after 8 days of curing and, beyond that period, no big alteration in the sample structure can be detected. The microstructure presented well-developed zeolite Na-A crystals with cubic-like morphology and a mean dimension of 1.5 µm. Na-A crystals seem to be surrounded by smaller nanometric crystals with the typical morphology of FAU zeolites. It seems that the porosity generated by foaming process promotes the zeolite nucleation mainly on the surfaces of the pores, whereas the struts remain amorphous. The cation exchange capacity resulted to be 3.32 meq/g. As regards the water softening capacity, the amorphous surface of the



geopolymeric struts can exchange cations to some extent, but also to adsorb them, while the crystalline zeolitic surface of the pores is mainly able to exchange cations, with a faster kinetic and a higher affinity toward magnesium.

The presence of a geopolymer backbone support and shape the zeolitic powder widening its technological application field. So, such specimens can be proposed as membranes or filters for ion exchange processes in aqueous solution.

*Keywords:* zeolite, membrane, geopolymer gel conversion

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I-28

## **CONTROLLING THE GEOPOLYMERIZATION REACTIONS BY MECHANICAL ACTIVATION OF SECONDARY RAW MATERIALS**

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Taking into account environmental considerations, such as decreasing CO<sub>2</sub> emission and the ecological footprint, the utilisation of secondary raw materials is essential for sustainable development. Industrial wastes and by-products, like power station fly ash, mining gangue, metallurgical slags, have good application possibilities mainly in the construction material industry, nevertheless, significant amount is landfilled due to their relatively low reactivity and heterogeneity. Hydraulic and geopolymerization properties of these materials can be tailored by mechanical activation achieving a higher added value product, for example supplementary cementitious materials (SCMs). The improved properties are higher specific surface area and desired particle size distribution (containing submicron size particles) as well as higher amount of reactive components that can be optimized by grinding. The objective of the present research is to investigate the effect of mechanical activation of various low-quality mineral bearing wastes by grinding on physico-chemical and mineralogical properties. It can be established that there are numerous techniques for mechanical activation of the above materials, e.g. planetary ball mill, vibratory mill or stirred media mill. However, most of the results reported in the literature are focusing on material related investigations without the discussion of the proper process circumstances. Nevertheless, beside this aspect, from energetic point of view the process related evaluation has even higher

importance in order to evaluate the feasibility of the developed technology. Based on this issue, another goal of the research is to compare the effect of mechanical activation of various waste materials on the geopolymer properties in different mills and circumstances and introduce energy utilization factors. The effect of mechanical activation of fly ash, slag and coal mining gangue on the geopolymerisation was investigated with FT-IR, SEM and XRD analysis. Finally, the relationship between material characteristics (particle size distribution, specific surface area, mineral composition, particle morphology), geopolymer properties (compressive strength, specimen density, microstructure) and process parameters (grinding energy, residence time, energy intensity, rotor velocity) was revealed.

O-1

## **MECHANOCHEMICAL vs. CHEMICAL SYNTHESIS IN THE PREPARATION OF $\text{YMnO}_3$ CERAMIC MATERIALS**

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Multiferroic materials simultaneously possess two or more ferroic orders, and enable a coupling interaction between them. The opportunity of controlling magnetic order via electric fields, and vice-versa, is captivating broad interest in developing multiferroic materials, for applications ranging from next generation data storage to sensing and energy conversion. The preparation of single-phase multiferroic materials is itself a very challenging task, involving innovative chemistry and/or combined synthesis methods.

$\text{YMnO}_3$  (YMO), as a representative of hexagonal family of rare earth manganites ( $\text{RMnO}_3$ ), possesses useful and interesting magnetic, ferroelectric and optical properties. Under this motivation, we investigated the impact of different synthetic paths on the properties of the  $\text{YMnO}_3$ , both powders and ceramic materials. Precursor YMO powders were obtained by mechanochemical and chemical synthesis.

In mechanochemical approach, milling of the starting mixture ( $\text{Y}_2\text{O}_3$  and  $\text{Mn}_2\text{O}_3$ ) in high energy planetary ball mill resulted in the preparation of the metastable orthorhombic YMO phase. After sintering under different conditions, ceramic material with hexagonal YMO as a major phase was obtained. Even though these samples had satisfying magnetic properties, their density under 90% of

theoretical value along with pronounced inter and intragranular cracks strongly influenced material's electric properties.

Polymeric precursor method, starting from yttrium and manganese citrate solutions, was used for the chemical synthesis. By optimization of sintering conditions of obtained polyphase powders, pure antiferromagnetic h-YMO ceramic materials were prepared, having densities higher than 95%. By comparing the ceramic materials prepared by means of two different methods, we could conclude that in case of  $\text{YMnO}_3$  chemical synthesis resulted in the preparation of material with better phase composition, microstructural, magnetic and ferroelectric properties.

O-2

## **COATING OF CERIUM OXIDE NANOPARTICLES WITH DIFFERENT CARBOHYDRATES**

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Cerium oxide nanoparticles ( $\text{nCeO}_2$ ) are biomaterials with numerous applications in biomedicine, fuel additives and electronics. Since their low stability in aqueous media limited their practical application, the aim of this study was to improve the suspension stability of  $\text{nCeO}_2$  by coating the particles. Glucose, monosaccharide, and levan and pullulan, microbial polysaccharides, were used as coating material. The coating was attempted under different synthesis conditions, by adding the carbohydrates during (direct coating) or after (subsequent coating) the synthesis of  $\text{nCeO}_2$ . X-Ray diffraction analysis, Fourier transform infrared spectroscopy (FT-IR), scanning electron microscopy (SEM) and transmission electron microscopy (TEM) were used for characterization of nanoparticles' powders. Measuring of hydrodynamic size, zeta potential and turbidity was used for

the estimation of nanoparticles' suspension stability in aqueous media. The success of subsequent coating with carbohydrates and the differences between coated nCeO<sub>2</sub> have been proven with FT-IR spectra. Turbidity measurement showed the best stability of levan- and glucose-coated nCeO<sub>2</sub> suspensions. It can be concluded that coating with carbohydrates improved the stability of the nCeO<sub>2</sub> suspension by decreasing the size of aggregated particles. The obtained results open new horizons for further ecotoxicity investigation and nCeO<sub>2</sub> application.

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O-3

## RELEVANT PROPERTIES OF GREEN SELF-COMPACTING CONCRETE

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The production of durable concrete with a high content of supplementing cementitious materials and recycled aggregate presents a step towards sustainability in the concrete industry. The paper presents the findings of the study, conducted on four series of concrete with self-compacting properties, which embodied recycled concrete aggregate, as a substitution for natural sand and gravel. Besides, this concrete possessed high content of fly ash, therefore qualifying as ecological (green) one. Particle packing method was used in the design of this concrete. Fresh properties included: density, slump flow, V-funnel, L-box and temperature, while compressive and tensile strengths were evaluated in the hardened state. Although certain difficulties in the application were recognized concerning the fast loss of workability in the fresh state, all of the tested mixtures exceeded the requirements of hardened structural concrete.

**Keywords:** self-compacting concrete, sustainability, physical and mechanical properties

O-4

## FIRST-PRINCIPLES INVESTIGATIONS OF ZnO/ZnS MIXED COMPOUNDS, POLYTYPISM AND (HETERO)STRUCTURES

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Zinc oxide (ZnO) is one of the most extensively investigated compounds in computational and experimental materials science, but in nature it only rarely occurs in pure form, as the mineral zincite. In contrast, zinc sulfide (ZnS) is very common and the main source of zinc found in nature, where it mainly appears as the mineral sphalerite. Both compounds have a large number of desirable properties for industrial applications, where they are successfully employed in electronics (e.g. LED, LCD, etc.), batteries and in optical materials, as well as additives to various materials, closely related to the structure–property relationships. As ZnS is the most common natural form of zinc, whereas ZnO is rarely found, it is not surprising that ZnO/ZnS solid solutions have not been found in nature. Recently, studies of ZnO/ZnS heterostructures and heterojunctions with various morphologies have been reported usually presenting improved physical and chemical properties for biosensors, electronics, magnetism, optics, catalysis, mechanics and electrochemistry. The main topic of this study are newly discovered ZnO/ZnS polytypes, which provide alternative structural arrangements of ZnO/ZnS compounds, including bulk crystal structures, various nanostructures, heterostructures and heterojunctions. In particular, pristine ZnO and ZnS compounds and mixed ZnO<sub>1-x</sub>S<sub>x</sub> compounds (x = 0.20, 0.25, 0.33, 0.50, 0.60, 0.66, and 0.75) have been investigated. First-principles calculations have been performed using Density Functional Theory (DFT), Local Density Approximation (LDA) and hybrid Heyd–Scuseria–Ernzerhof (HSE06) functionals. A multitude of possible stable polytypes for ZnO/ZnS compounds have been discovered creating new possibilities for synthesis of new materials with improved physical and chemical properties.

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O-5

## FIRST PRINCIPLE INVESTIGATION OF $\text{Al}_{1-x}\text{B}_x\text{N}$ SOLID SOLUTION

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Aluminum nitride (AlN) is a wide band gap semiconductor and ceramic material with high melting point, high thermal conductivity, electrical resistivity and thermal shock resistance. Boron nitride (BN) is a heat and chemically resistant refractory compound, used as HT and LT lubricants, in alloys, plastics, rubbers and other materials, in nanotechnology and laser printers. Because of excellent thermal and chemical stability, BN ceramics are traditionally used as parts of high-temperature equipment. AlN crystallizes in hexagonal wurtzite type of structure with a space group  $P6_3mc$  (no. 186) at standard conditions. On the other hand, boron nitride exhibits  $h$ -BN structure type with space group  $P6_3/mmc$  at ambient conditions. Additionally, wide energy bands gaps of 6.2 and  $\sim 5.2$  eV have been observed in the aluminum nitride and  $h$ -BN, respectively. In this work we have conducted first principle investigation of solid solutions with general formula  $\text{Al}_{1-x}\text{B}_x\text{N}$  ( $x = 0; 0.125; 0.25; 0.375; 0.5; 0.625; 0.75; 0.875$  and 1). Investigated structures were generated using data mining [1,2], while compositions were obtained using supercell and PCAE approach [3,4]. Local structure optimization was performed using hybrid B3LYP (Becke, three-parameter, Lee-Yang-Parr) exchange-correlation functional. Each of the B doped AlN compositions were investigated for structure stability, resulting in energy vs. volume ( $E(V)$ ) curves. In this way, we address new possibilities for improving stability and structural properties of BN/AlN based ceramic materials, which might have great technological and industrial applications.

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O-6

## THE INORGANIC CRYSTAL STRUCTURE DATABASE (ICSD)

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The inorganic crystal structure database (ICSD) is the most comprehensive source for high-quality crystal structures. In recent years, the information content has been significantly expanded, especially for materials researchers. Important improvements include the introduction of keywords for material properties and the extension of the scope of ICSD to include theoretically calculated structures. Organo-metallic structures are also recorded if inorganically relevant material properties or inorganic applications are given. These extensions of the database offer new possibilities for data-mining approaches.

In this talk we will show how these new features can be used in ICSD and what possibilities they offer. Furthermore, an outlook on the planned further development of ICSD will be given.

O-7

## MULTIFUNCTIONAL COMPOSITE COATINGS WITH SELF-CLEANING AND ANTIMICROBIAL PROPERTIES CONTAINING OXIDE NANOPOWDERS

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Recently, great attention has been focused on multifunctional composite coatings incorporating metal oxide nanostructures with photocatalytic and antimicrobial properties. Such coating formulations have potential applications in the protection of buildings and monuments from environmental pollutants and biodegradation.

Phase-pure TiO<sub>2</sub> (anatase form) and MgO (periclase form) nanopowders were obtained by sol-gel synthesis starting from titanium alkoxides and, respectively,

magnesium nitrate followed by thermal treatment. The oxide powders were dispersed in hydrophobically modified polyacrylate (NaPAC<sub>16</sub>) polymer aqueous solutions and coatings were deposited on glass slides. The obtained powders and composite coatings have been characterized by: TG/DTA, BET specific surface area and porosity, DLS, FT-IR, XRD, AFM, SEM and Spectroelipsometry. Coating hydrophobicity was verified by contact angle measurements. Photocatalytic and antimicrobial activity of the powders and composite coatings were tested.

*Acknowledgements:* This work was supported by a grant of the Romanian Ministry of Research and Innovation, CCCDI-UEFISCDI, project number PN-III-P1-1.2-PCCDI-2017-0476/51PCCDI/2018, within PNCDI III.

O-8

## **SYNTHESIS AND QUANTIFICATION OF KAOLINITE NANOSCROLLS**

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Nowadays, the exfoliation of kaolinite through multi-step intercalation is an important research field, because the kaolinite plates converted into nanoscrolls can be applied in advanced nanocomposite and nanohybrid materials. These halloysite-like nanoscrolls can be produced by multiple intercalation and deintercalation steps. During this treatment, kaolinite layers can be exfoliated, i.e. they can be separated into individual double layers. To compensate stresses due to misfit of tetrahedral and octahedral sheets, the exfoliated kaolinite layers curl and frequently roll up to form nanoscrolls.

Our high-efficient solvothermal technique was optimized for laboratory condition; therefore, the increase of produced quantities is very important research topic from the industrial point of view. Furthermore, an appropriate quantification technique of produced nanoscrolls is missing yet. In this work, we investigated the multi-step intercalation of kaolinite with increasing the produced quantities using solvothermal methods. Kaolinite-urea precursors were used to produce directly kaolinite-cetyltrimethylammonium chloride (kaolinite-CTAC) complexes, which were suitable for the exfoliation of kaolinite and the formation of kaolinite nanoscrolls. The quantity of kaolinite nanoscrolls was established using X-ray diffraction (XRD) and transmission electron microscopy (TEM).



O-9

## PREPARATION OF Ag DOPED CERIA CERAMICS

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Nanosized Ag-doped ceria ( $\text{Ce}_{1-x}\text{Al}_x\text{O}_{2-\delta}$ ) powders ( $0 \leq x \leq 0.04$ ) were obtained by self-propagating room temperature reaction. X-ray diffraction analysis and field emission scanning microscopy results showed that the doped samples are solid solutions with fluorite-type structure and all powders were nanometric in size. The average size of  $\text{Ce}_{1-x}\text{Al}_x\text{O}_{2-\delta}$  particles lies about 4 nm. Raman spectra revealed an increase in the amount of oxygen vacancies with the increase of Ag concentration. This increasing results in a narrowing of the bandgap of  $\text{CeO}_2$ . The photocatalytic performances of the Ag-doped ceria solid solutions were evaluated by decomposing an organic dye, crystal violet under UV irradiation. The Ag-doped ceria solid solutions exhibit significantly better photocatalytic activity than the pure  $\text{CeO}_2$  and commercial  $\text{TiO}_2$ . The densification process was studied by isothermal and microstructural development by scanning electron microscopy. By controlling the processing variables, it was possible to obtain high density samples with a homogeneous microstructure at low-temperature. A closer examination of silver doped ceria indicated that silver affects sintering by producing a liquid at the ceria grain boundaries. Due to this liquid phase sintering, it was possible to produce dense nanostructured ceria at lower temperatures.

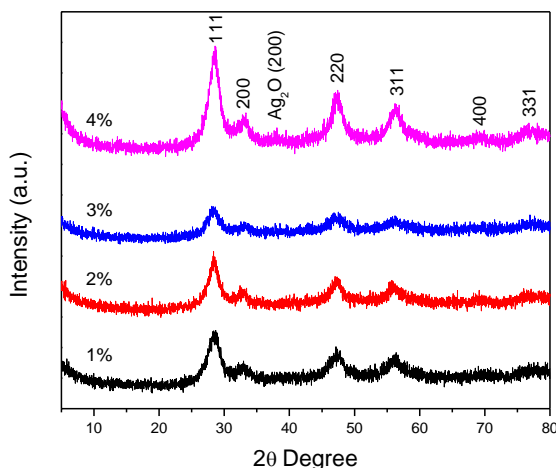


Figure 1. XRD patterns of obtained Ag doped ceria powders at room temperature

O-10

## FORMATION OF METAL POWDERS BY ELECTROLYSIS: COMPARISON OF MORPHOLOGICAL AND CRYSTALLOGRAPHIC CHARACTERISTICS

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Morphology of electrolytically produced metal powders depends on applied regimes and parameters of electrolysis, and of affiliation to determined group of metals [1]. Following the values of the exchange current density ( $j_0$ ), melting point ( $T_m$ ) and overpotential for hydrogen discharge ( $\eta(\text{H}_2)$ ), metals are classified into three groups: (a) *normal metals* (Pb, Ag(basic electrolytes), Sn, Zn, Cd); this group of metals is characterized by the high both  $\eta(\text{H}_2)$  and  $j_0$ , and by low  $T_m$ , (b) *intermediate metals* (Cu, Ag(complex electrolyte), Au); this group of metals is characterized by moderate  $T_m$  and medium  $j_0$ , and (c) *inert metals* (Pt, Fe, Co, Ni); this group of metals is characterized by the both low  $j_0$  and  $\eta(\text{H}_2)$ , and by high  $T_m$  [2].

In this study, comparison of morphological and crystallographic characteristics of electrolytically produced silver and copper powders was presented. For these purpose, silver powders were electrolytically synthesized from nitrate (basic) and ammonium (complex) electrolytes, while copper powders were synthesized using sulphate electrolyte. Depending on overpotential of electrolysis, either the needle-like or the 2D fern-like dendrites of Ag were formed from the nitrate electrolyte [3]. Irrespective of overpotential of the electrodeposition, the 3D pine-like dendrites constructed from small agglomerates of approximately spherical grains were formed from the ammonium electrolyte. In the case of copper, the shape of particles depended on the amount of generated hydrogen as a parallel reaction to Cu electrolysis in the powder production range. The 3D pine-like dendrites were formed with an amount of evolved hydrogen insufficient and the cauliflower-like particles (the honeycomb-like structures) were formed with amount evolved hydrogen sufficient to achieve strong effect on hydrodynamic conditions in the near-electrode layer. The both types of Cu particles were constructed from small agglomerates of approximately spherical grains. X-ray analysis of the produced powders showed that the preferred orientation of the particles changed from the strong (111) for the needle-like dendrites of Ag to almost random oriented crystallites in approximately spherical grains of Ag and Cu. Morphologies of Ag and Cu particles were successfully correlated with their crystal structure.

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O-11

**SPIN-COATING DEPOSITION OF DENSE  $\text{BaZr}_{0.7}\text{Pr}_{0.1}\text{Y}_{0.2}\text{O}_{3-\delta}$   
ELECTROLYTE THICK FILMS ON NI-BASED ANODES  
FOR IT-SOFCs**

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High temperature proton conducting  $\text{BaZr}_{0.7}\text{Pr}_{0.1}\text{Y}_{0.2}\text{O}_{3-\delta}$  (BZPY10) thick films are deposited on cermet anodes made of  $\text{NiO-BaZr}_{0.7}\text{Pr}_{0.1}\text{Y}_{0.2}\text{O}_{3-\delta}$  (NiO-BZPY10) using spin-coating technique. BZPY10 powders are prepared by the citrate–nitrate auto-combustion (CNA) method and the cermet anodes are prepared by milling of BZPY10 and NiO in acetone. The parameters of spin-coating are optimized; the deposition time is varied between 30 and 120 s and the rotation speed is varied between 3000 and 6000 rpm. The anode substrates and electrolyte films are co-sintered in the range 1300–1400 °C for 3–5 h to obtain a dense electrolyte film and to examine the sinterability of BZPY10 electrolyte film. Also, during this single heat treatment, the aim was to maintain a suitable porosity in the anode and to obtain large electrolyte grains keeping the grain boundary resistance low. The samples of anode-electrolyte bi-layer are characterized by field emission scanning electron microscopy (FE-SEM). A prototype fuel cell is prepared depositing a composite  $\text{La}_{0.8}\text{Sr}_{0.2}\text{Co}_{0.8}\text{Fe}_{0.2}\text{O}_3$  (LSCF)– $\text{BaZr}_{0.5}\text{Pr}_{0.3}\text{Y}_{0.2}\text{O}_{3-\delta}$  (BZPY30) cathode on the co-sintered half-cell. Fuel cell tests of the prototype single cells are performed in the range of temperatures 500–650 °C in the wet  $\text{H}_2$  atmosphere.

O-12

## **HUMIDITY SENSOR BASED ON MESOPOROUS SnO<sub>2</sub> FABRICATED VIA NANOCASTING TECHNIQUE**

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In this contribution, the mesoporous SnO<sub>2</sub> was fabricated via nanocasting, where the hydrothermally processed silica KIT-5 with a high specific surface area of 610 m<sup>2</sup>/g and pore volume of 0.72 cm<sup>3</sup>/g was used as a hard template. Following the two precursor loading/calcination steps of the wet impregnation process, the appropriate amount of the Sn- precursor solution was used to fill up 15 % of the total pore volume of the silica template with SnO<sub>2</sub>. This synthesis route with a template etching by 2M NaOH solution resulted in nanocast SnO<sub>2</sub> with Brunauer-Emmett-Teller specific surface area of 33 m<sup>2</sup>/g, where SnO<sub>2</sub> nanoparticles of 8–10 nm formed the ordered domains along with fractions of disordered regions, as confirmed by the transmission electron microscopy (TEM). Based on the Barrett-Joyner-Halenda model from the desorption branch of the N<sub>2</sub> adsorption/desorption isotherms, the pore size of SnO<sub>2</sub> is centered at 8.6 nm, demonstrating quite open and accessible pore structure of the material. Wide-angle X-ray diffraction (XRD) measurement confirmed the formation of the tetragonal SnO<sub>2</sub> phase. Because of the low Si content after the template etching (< 0.5%, confirmed by EDS analysis), formation of substantial amounts of SnSiO<sub>3</sub> can be excluded, and no evidence for such phase was found in the XRD.

The as prepared SnO<sub>2</sub> nanocast was further used to fabricate a few micron thick film by the doctor blade technique on alumina substrate provided with interdigitated Pt/Ag electrodes. The sensor response of the film towards humidity was tested measuring the change of the complex impedance of the sample exposed to a humid climate chamber environment with the relative humidity (RH) ranging from 40% to 90% at 25 °C and from 30% to 90% at 50 °C. The value of impedance measured at 100 Hz and 25 °C was reduced 132 times within the RH range of 40 % to 90 %, while it tended to decrease in a moderate manner at 50 °C under the same frequency and RH range. The film exhibited remarkably rapid response (4 s) and quick recovery time (6 s) when exposed to RH change from 37% to 90% at 25 °C. Such a fast response/recovery time and relatively low hysteresis of 4% observed under 50 % RH and 25 °C indicate the promising potentials of nanocasted SnO<sub>2</sub> to be used as an active layer for humidity sensors.

O-13

## **PROCESSING OF $\text{Bi}_{0.5}\text{Na}_{0.5}\text{TiO}_3$ BASED PIEZOELECTRIC CERAMICS**

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Due to the large pollution caused by burning of fossil fuels, technology is developing in the direction of using alternative sources of energy. Solar panels, wind turbines and geothermal energy are already being used intensively, but energy harvesting based on piezoelectric materials is attracting a lot of attention. The most efficient are Lead zirconate titanate ( $(\text{Pb}(\text{Zr}_x\text{Ti}_{1-x})\text{O}_3)$ ) based devices, but due to ecological problems, they are being replaced with lead-free materials. Bismuth sodium titanate,  $\text{Bi}_{0.5}\text{Na}_{0.5}\text{TiO}_3$  (BNT) based materials are recognized as a good substitute owing to their good functional properties and high Curie temperature. Piezoelectric properties of BNT materials can be improved by modification with barium titanate ( $\text{BaTiO}_3$ ) because of the existence of morphotropic phase boundary (MPB) which is characterized by the coexistence of two phases.

Pure  $\text{Bi}_{0.5}\text{Na}_{0.5}\text{TiO}_3$  and  $\text{Bi}_{0.5}\text{Na}_{0.5}\text{TiO}_3$  doped by  $\text{Ba}^{2+}$  ions powders were prepared by wet chemical synthesis. The aim of this research was to examine the influence of addition of  $\text{Ba}^{2+}$  ions (up to 10 at.%) and different processing parameters on the phase composition, sinterability and dielectric properties of material. Bismuth nitrate pentahydrate ( $\text{Bi}(\text{NO}_3)_3 \cdot 5\text{H}_2\text{O}$ ), titanium butoxide ( $\text{C}_{16}\text{H}_{36}\text{O}_4\text{Ti}$ ), sodium hydroxide ( $\text{NaOH}$ ) and barium nitrate ( $\text{Ba}(\text{NO}_3)_2$ ) were used as starting materials. The obtained powders were dried, pressed into pills and finally sintered at different temperatures up to 1200 °C. The obtained samples were characterized by X-ray diffraction (XRD), Raman spectroscopy, Scanning electron microscopy and dielectric measurements.

O-14

## THE INTERPLAY OF PHASES, STRUCTURAL DISORDER AND DIELECTRIC BEHAVIOR IN Al DOPED BiFeO<sub>3</sub>-BaTiO<sub>3</sub> CERAMICS

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Al doped BiFeO<sub>3</sub>-BaTiO<sub>3</sub> (BFA-BT) systems with a defined composition were prepared by solid-state method. The enhanced spontaneous and remnant polarization were achieved in BiFe<sub>0.970</sub>Al<sub>0.030</sub>-BaTiO<sub>3</sub> with 36.8  $\mu\text{C}/\text{cm}^2$ , 31.5  $\mu\text{C}/\text{cm}^2$ , respectively. From SEM and XRD analyses, the high-density of the ceramics and the high lattice parameters ratio  $c_T/a_T$  traducing large distortions of the rhombohedral phase play a dominant role in the enhanced piezoelectric properties. The high polarization and large strain were achieved in the BF<sub>0.970</sub>A<sub>0.030</sub>-BT system. <sup>57</sup>Fe Mössbauer spectra revealed the large disorder of Fe<sup>3+</sup> at B sites preferentially occupied by more Al<sup>3+</sup> doping ions, forming the diffusive phase transition for dielectric behaviors in samples. Grain and grain-boundary effects were pointed out from the dielectric modulus and a related thermal evolution. AC capacitances indicated two relaxation processes marked by the grains and interfaces involved in the polycrystalline ceramics for highly doped systems. The work will be significant to illuminate the interplay between structures and properties in ferroelectric materials.

O-15

## **TEMPERING RECIPES OF THE CHALCOLITHIC POTTERY: CASE STUDIES FROM EASTERN ROMANIA**

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This study is part of a larger project focused on identifying the main technological characteristics of a special category of pottery identified within the Cucuteni culture, labelled Cucuteni C (4300–3500 cal BC) and its relationship with the Cucuteni painted and unpainted ware. The Cucuteni C ware represents a highly debated ceramic category since its first mention at the beginning of the 20<sup>th</sup> century, when it was interpreted as originating from the Eurasian steppe region. Although, it was highlighted among the Cucuteni ceramic assemblages based on its specific temper (e.g. the use of crushed pottery fragments - called “grog” - and crushed shells) or decorative style (e.g. cord-impressed and comb-incised ornamentation) its technological complexity was never assessed.

A multi-analytical approach was applied to grog and shell tempered ware selected from five archaeological sites located in Eastern Romania. The ceramic samples were first thin-sectioned and analyzed by light polarized microscopy for identifying pottery paste types based on the amount, nature, grain-size, degree of sorting and shape of inclusions. Then, the pottery matrix and inclusions were investigated by Scanning Electron Microscopy coupled with Energy-dispersive X-ray spectroscopy (SEM-EDX) for determining the major elements and microstructural features. For identifying the firing history of the ceramic ware, we have performed X-ray diffraction (XRD) analysis.

The combined use of point chemical and microstructural analyses allowed for establishing differences in composition between the pottery matrix and the added temper from the different sites studied. It has also evidenced that some grog fragments have a similar composition to that of the matrix. Furthermore, the comparison between the chemical characteristics of the grog-tempered ware (matrix and inclusions) and our previously analyzed Cucuteni painted ware identified in the same site evidenced a high degree of similarity for some of the pottery samples prompting to a similar provenance [1, 2].

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P-1

## **HYDROGEN PEROXIDE-ASSISTED ROUTE FOR NANOCRYSTALLINE WO<sub>3</sub> SYNTHESIS WITH EXCELLENT SENSING RESPONSE**

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Tungsten oxide (WO<sub>3</sub>) is a wide band gap semiconductor and it is widely used in solar cells, supercapacitors, photochromic, gas chromic and electrochromic devices, humidity sensors, as photocatalyst for enhanced water splitting and water purification. A special attention is currently paid to the sensing properties of WO<sub>3</sub>. In particular WO<sub>3</sub> demonstrates the highest sensitivity and selectivity towards NO<sub>2</sub>, over a wide range of temperatures. It has been repeatedly shown that the WO<sub>3</sub> sensing properties are affected by several key parameters including phase composition, microstructure and the temperature of annealing, visible light illumination also affects its sensing properties.

The functional characteristics of tungsten oxide are largely determined by the synthesis method and so the search for the new approaches to WO<sub>3</sub> synthesis or significant modification of existing ones still remains the most crucial task. There are few reports concerning WO<sub>3</sub>-based NO<sub>2</sub> sensors preparation by precipitation, gas transport, thermal decomposition, thermal oxidation or high temperature anodization of metallic tungsten, electrospinning and low frequency electrophoretic deposition. Most of these methods are multistage and time-consuming. Varying synthetic conditions within a single synthetic approach, one can easily obtain two-phase composite materials containing several WO<sub>3</sub> polymorphs, thus reaching the high sensor properties inherent to traditional composites.

Here, we report excellent NO<sub>2</sub>-sensoric properties of tungsten oxide nanoparticles prepared by a facile procedure which includes dissolution of metallic tungsten in hydrogen peroxide with subsequent low-temperature (400°C) heating. We found that the sensor response towards NO<sub>2</sub> registered in this work is at the highest achieved levels. The most intriguing feature of the material obtained is a high reproducible sensor signal at room temperature being more than 100 times higher than reported previously for WO<sub>3</sub>. The probable reason for such a high sensor response is the presence of two WO<sub>3</sub> polymorphs ( $\gamma$ -WO<sub>3</sub> and h-WO<sub>3</sub>) in the material synthesized by a peroxide-assisted route.

*Acknowledgment:* This work was supported by the Russian Science Foundation (Project No. 18-73-10150).



P-2

## THE POTENTIAL OF HYBRID GEOPOLYMER COMPOSITES

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Hybrid geopolymers represent a new class of composite materials formed by incorporating organic polymer into a geopolymer matrix. The properties of hybrid geopolymer depend on the addition of organic phase and the starting raw material composition (concentration of NaOH in alkaline activator, Si/Al mass ratio and solid/liquid mass ratio). In addition to these relevant parameters, this paper examines the synthesis conditions of these materials through the influence of the type, amount and manner of adding organic modifiers (commercial epoxy resins and 3-(methoxyl) propyl methacrylates) on forming the structure with significantly reduced pore distribution and decreased pore size, which exhibits good mechanical properties.

The purpose of this research is to define the optimal conditions of the hybrid geopolymers' synthesis through the examination of relevant parameters. Expected improvement of mechanical properties was confirmed through values of compressive strength. Characterization of hybrid geopolymer composites was performed by XRD analysis, DRIFT spectroscopy and SEM analysis.

**Keywords:** hybrid geopolymer composites, XRD, SEM, DRIFT spectroscopy, compressive strength

P-3

## SYNTHESIS, CHARACTERIZATION AND PHOTOCATALYTIC PROPERTIES OF $\text{LaNiO}_3$ -BASED POWDERS

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Lanthanum nickelate ( $\text{LaNiO}_3$ , LNO) belongs to the group of materials with perovskite-type structure and it crystallizes in rhombohedrally distorted perovskite lattice. This material exhibits interesting electrical, magnetic, optical and catalytic properties and it is suitable for various applications. Still, the preparation of single phase LNO is difficult, because at temperatures above 850 °C it decomposes into the lower oxides with formula  $\text{La}_{n+1}\text{Ni}_n\text{O}_{3n+1}$  ( $n = 3, 2, 1$ ) and  $\text{NiO}$ .

In this work we present the synthesis of pure and Nb doped LNO powders,  $\text{LaNi}_{1-x}\text{Nb}_x\text{O}_3$  ( $x = 0.000, 0.005, 0.010$ ) prepared from mechanochemically activated oxide precursors –  $\text{La}_2\text{O}_3$ ,  $\text{NiO}$  and  $\text{Nb}_2\text{O}_5$ . For this experiment, precursor powders homogenized in isopropyl alcohol were dried and mechanochemically activated in the planetary ball mill for 3 h. As-prepared powders were calcined at 700 °C for 3 h in air and further analyzed by X-ray diffraction analysis (XRD), Transmission electron microscopy (TEM), Scanning electron microscopy (SEM) and UV-Vis spectroscopy. Photocatalytic activity in visible light was investigated.

The XRD analysis of undoped LNO revealed the existence of rhombohedral  $\text{LaNiO}_3$  and small amount of  $\text{NiO}$  phase. The doped samples, apart from LNO, contained products of thermal decomposition – layered oxides and  $\text{NiO}$ . TEM and HRTEM analyses of undoped LNO revealed the presence of agglomerated particles with single particle size being in the range of 20–40 nm. Doping with Nb led to decrease of agglomeration process and allowed better dispersion between particles of LNO based powders. Calculated band gaps were 1.12 eV, 0.89 eV and 0.87 eV for  $x = 0.00, 0.005, 0.010$ . The absorption spectra indicated photocatalytic degradation of Reactive Orange 16, textile dye used as a model in these experiments.

P-4

## **INFLUENCE OF Co<sup>2+</sup> IONS ON PHOTOCATALYTIC PROPERTIES OF MgFe<sub>2</sub>O<sub>4</sub> FERRITES**

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In this work, spinel magnesium cobalt ferrites (Co<sub>x</sub>Mg<sub>1-x</sub>Fe<sub>2</sub>O<sub>4</sub>, x = 0.0, 0.1, 0.3, 0.5, 0.7, 0.9) were synthesized by a sol-gel combustion method. Magnesium nitrate, cobalt nitrate and iron nitrate were used as oxidizers and citric acid was used as a reducing agent. The effects of cobalt ions on structural and morphological properties were investigated and characterized by X-ray diffraction (XRD), Raman spectroscopy, Field emission scanning electron microscope (FESEM) and Fourier transform infrared (FT-IR) spectroscopy. A cubic spinel structure formed with a varied distribution of cobalt and magnesium ions on tetrahedral and octahedral sites that depended on their content. All ferrite powders consisted of multigrain agglomerates. Optical properties were investigated by UV- vis spectrophotometry. The photocatalytic activity of as prepared samples was evaluated by measuring the rate of photodegradation reaction of methylene blue (MB) under visible light irradiation. After 240 min, compared to other samples, the sample labeled as Co<sub>0.1</sub>Mg<sub>0.9</sub>Fe<sub>2</sub>O<sub>4</sub> showed the best rate of photodecomposition of MB resulting in reduction of 90% of its initial concentration.

P-5

## REMOVAL OF NICKEL IONS FROM AQUEOUS SOLUTIONS BY ADSORPTION ONTO NATURAL SORBENTS

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Nickel has many useful applications in our life, but it is harmful if discharged into natural water resources. Ni(II) is present in the effluents of silver refineries, electro-plating, zinc base casting and storage battery industries [1]. Contact with nickel compounds (both soluble and insoluble) can cause a variety of adverse effects on human health. The most important and frequent are nickel allergy, lung fibrosis, cardiovascular and kidney diseases, and lung and nasal cancers [2,3]. Various conventional methods were designed and used to remove nickel ions from aqueous solutions. Adsorption process is commonly applied because of its ease of application as well as its cost effectiveness. The removal of nickel ions from aqueous solutions using the adsorption process onto natural slovak zeolites from deposits Kučín and Nižný Hrabovec (Slovakia) and bentonites from deposits Jelšový potok and Liesko-vec (Slovakia) has been investigated. The adsorption experiments were carried out at 30 °C under batch process with initial concentration Ni(II) ions and time as the variables. A flame atomic absorption spectrometer Avanta  $\Sigma$  (GBC) was used for measuring the nickel concentration before and after adsorption. The results of nickel ions adsorption experiments were best fitted by Langmir adsorption isotherm for all investigated adsorbents. The Langmuir maximum adsorption capacity of the adsorbents was from 3.30 to 24.81 mg g<sup>-1</sup>. Adsorption was very fast at low coverage and equilibrium was approached within 20 min. The results suggested that natural bentonites are more suitable than zeolites and can be used as a adsorbent material for recovery and adsorption of Ni(II) ions from aqueous solutions. Comparing the measured results for used bentonites is evident that for the removal of Ni(II) ions from aqueous solutions is more suitable the bentonite from Jelšový potok. Both types of zeolites that we used at in this study have similar adsorption properties.

*Acknowledgment:* This work was supported by the Slovak Grant Agency VEGA [1/0291/19].

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P-6

## CHEMICALLY MODIFIED NANO-STRUCTURED $\gamma$ -ALUMINA IN PROCESS OF BIODIESEL PRODUCTION

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The main benefits of using biodiesel as the candidate for a diesel fuel substitution are that it is non-toxic, bio-degradable; it produces reduced volumes of harmful gases emissions and can be used without modifying existing (motor) engines. Biodiesel is most commonly produced by transesterification of vegetable oils (in this case, sunflower oil). Heterogeneous catalysis is in recent focus of research for biodiesel production from vegetable oils because of numerous advantages such as: easy phase separation and reuse of catalysts. The aim of this study was the preparation of nanostructured  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> by using improved sol-gel procedure, synthesis of the KI/Al<sub>2</sub>O<sub>3</sub> catalyst and testing its activity in the transesterification of sunflower oil with methanol. The effects of different process parameters (different catalyst loading, methanol to oil molar ratio, stirring rate, and co-solvent use) were considered. The results show that the potassium iodide incorporation into/onto the structure of nano-structured  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> significantly influences textural and structural properties of the catalyst as well as its total surface basic strength and positively affects the activity of the catalyst in the reaction of transesterification of sunflower oil with methanol. The surface properties of the catalyst have an essential impact on its catalytic performance, the impregnation of alumina with potassium iodide resulted in the formation of (relatively) strong base catalytically active sites.

Under relatively mild process conditions and relatively short reaction time (methanol to oil molar ratio, 12:1; reaction time, 180 min; catalyst loading, 2.5 wt.% and reflux temperature) the usage of the KI/Al<sub>2</sub>O<sub>3</sub> catalyst resulted in very high conversion to fatty acids methyl esters (*i.e.*, 99.99%).

*Acknowledgement:* The authors wish to thank to the Ministry of Education, Science and Technological Development of the Republic of Serbia (Project III 45012 and TR 34008) for financial support.

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P-7

## **GEOPOLYMER- DOPED BY CeO<sub>2</sub> AS SOLID ELECTROLYTE**

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For the first time, geopolymer - doped by ceria was synthesized as potential low cost material for application in solid oxide fuel cells operating at intermediate temperature (IT-SOFC). The new materials were obtained by alkali activated metacaolin (calcined clay) in the presence of CeO<sub>2</sub> powders. Beside the commercial CeO<sub>2</sub> powder (GP\_CeO<sub>2</sub>\_com), as a source of ceria, a two differently synthesized CeO<sub>2</sub> powders also were used: CeO<sub>2</sub> synthesized by modified glycine nitrate procedure (GP\_CeO<sub>2</sub>\_ MGNP) and self-propagating reaction at room temperature (GP\_CeO<sub>2</sub>\_ SPRT). All produced geopolymers-CeO<sub>2</sub> were characterized by XRD, FTIR, DTA-TGA, FESEM, MALDI and EIS analysis. Results show that geopolymer-CeO<sub>2</sub> was successfully obtained in form of composite with good electrical properties ( $1.03 \times 10^{-2} \Omega^{-1} \text{cm}^{-1}$  for GP\_CeO<sub>2</sub>\_ MGNP at 600 °C and  $9.53 \times 10^{-3} \Omega^{-1} \text{cm}^{-1}$  for GP\_CeO<sub>2</sub>\_ SPRT at 650 °C). This indicates that geopolymer-CeO<sub>2</sub> presents the right features for use as a solid electrolyte.

**Keywords:** geopolymer, cerium (IV)-oxide, ion conductivity

P-8

## **METAKAOLIN-BASED INORGANIC POLYMER SYNTHESIS USING ALKALINE ACTIVATOR**

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This paper reports an environmental friendly, energy saving, clean technology which conserve the natural environment and resources using a metakaolin as a precursor for synthesis of inorganic polymer (geopolymer). The influence of alkali activation, i.e. different concentration of NaOH as a component of alkali activator mixture on the process of geopolymerization of metakaolin is investigated. Also, process of aging time of geopolymer samples at 7<sup>th</sup>, 14<sup>th</sup>, 21<sup>st</sup> and 28<sup>th</sup> days is followed by some analytical methods. The structure of metakaolin and metakaolin-based inorganic polymers and their physicochemical properties were studied using X-ray diffraction (XRD), Fourier transformation infrared spectroscopy (FTIR), and after 28<sup>th</sup> days using scanning electron microscopy (SEM) with energy dispersive spectroscopy (EDS) on the surface of the samples. The FT-IR results show a shift of the Si-O or Si-O-X (X=Si, Na, or H) bands as the molarity of activator increasing during geopolymerization process. Scanning electron microscopy (SEM) provides excellent insight into the morphology of inorganic polymers. Structural reorganization of geopolymer samples occurs during the curing or aging in accordance with a geopolymerization mechanism.

P-9

## **A NEW DENTAL MATERIAL ON THE CALCIUM ALUMINATE CEMENT**

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A new dental material based on calcium aluminate cement was synthesized and characterized in this study. Physico-chemical and mechanical properties of the material were investigated before and after various periods of hydration. Phase analysis of the material was performed by X-ray diffraction analysis, while morphological analysis was performed by scanning electron microscopy equipped with EDS which revealed elemental composition of the material. Investigations of mechanical properties showed that this new material possessed good mechanical properties and short setting time. Additionally, cytotoxicity and genotoxicity of the material were investigated. The obtained results suggest that this material have potential for application in dental practice.

P-10

## **INFLUENCE OF Ag DOPING ON THE CRYSTAL STRUCTURE AND MAGNETIC PROPERTIES OF CuO NANOPOWDERS**

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The influence of Ag doping on the crystal structure and magnetic properties of CuO nanopowders was investigated. Nanoparticles of copper-silver oxide solid solutions with composition  $\text{Cu}_{1-x}\text{Ag}_x\text{O}$  ( $x=0.01-0.05$ ) were successfully produced by self-propagating room temperature synthesis using reaction between metal nitrates and sodium hydroxide. Prepared powders were calcinated at 700 °C for 2 h. The diffraction pattern was recorded at room temperature and atmospheric pressure without any re-heating of the sample. A fitting refinement procedure using the



Rietveld method was performed which showed the incorporation of  $\text{Ag}^{3+}$  ions in the  $\text{CuO}$  crystal lattice, where they substitute  $\text{Cu}^{2+}$  ions. Magnetic behaviour of synthesized materials was investigated by SQUID magnetometer in temperature interval 2–400 K. It is known that copper(II) oxide exhibits ferroelectricity driven by magnetic order at temperature as high as 230 K [1]. Multiferroic phase is present above the first order phase transition at  $T_{N1} = 213$  K and exists up to the subsequent first order phase transition  $T_{N2} = 230$  K [1,2]. It was shown that disorder in the form of impurities can stabilize the ferroelectric phase [2]. This was our motivation to dope  $\text{CuO}$  with  $\text{Ag}$  in order to further improve its multiferroic properties. In  $\text{Cu}_{1-x}\text{Ag}_x\text{O}$  small changes of magnetic properties were observed if compared to  $\text{CuO}$ .

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P-11

### **IMPROVEMENT OF PHYSICAL AND MECHANICAL PROPERTIES OF GEOPOLYMER THROUGH ADDITION OF ZIRCON**

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To improve physical and mechanical properties of geopolymer, an attempt to incorporate zircon- $\text{ZrSiO}_4$  with aluminum silicates in the matrix was addressed and we studied the effect of incorporated zircon ( $\text{ZrSiO}_4$ ) with aluminium silicates on the mechanical properties of a geopolymer. We have expected improved structural and chemical properties of obtained four prepared geopolymers with different weight percent of incorporated zirconium. These geopolymer pastes were prepared from Serbian kaolin with alkali activators and various methods for materials`

characterization were employed for their characterization in addition to the bulk density and apparent porosity and the compressive strength of prepared geopolymers. Characterization of obtained geopolymers was performed with X-ray diffraction (XRD), Scanning electron microscopy (SEM-EDS), Fourier transform infrared spectroscopy (FTIR) and matrix-assisted laser desorption ionization time-of-flight mass spectrometry (MALDI-TOF). In summary, results indicated that no interconnected phases were formed between added zircon and starting aluminum silicates or alkali activators. The presence of zircon up to 10 g/100 g metakaolin, led to the improvement of the microstructure of prepared geopolymer, whereas the maximum obtained compressive strength value was 70.15 MPa for the sample that contains 10 g zircon. Addition of higher amount of zircon (20 g/100 g metakaolin) hinders the progress of geopolymerization reaction to take place and consequently decreases the compressive strength.

P-12

## **CuO-BASED NANOPATELETS FOR HUMIDITY SENSING APPLICATION**

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Determination and monitoring of humidity level is of great importance because water is one of essential components of the living organisms and materials used by people. Metal oxides are the most popular materials used as sensing elements for humidity sensors, due to their excellent thermal and environmental stability, high mechanical strength, wide range of working temperature, low fabrication cost and robustness in practical applications. Humidity sensing ability of metal oxide based ceramic materials can be enhanced by doping with metal cations.

In this work, we present hydrothermal method for preparation of pure and Mg-doped CuO nanoplatelets and investigate their sensing properties towards humidity. The proposed method involves autoclaving of copper(II)-acetate solution under autogenous pressure in alkaline conditions, with different concentrations of Mg-dopant (0, 2.5, 5 and 10 mol%). We have performed thorough structural and optical investigations of as synthesized material (TEM, XRD, SAED, UV-VIS-NIR). Furthermore, we have processed obtained powders into functional thick films using

doctor blade technique, and their sensing properties were tested in wide range of temperatures (25, 50, 75 °C) and relative humidities (40–90%), resulting with strong response and promising response/recovery times.

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## CHEMICAL STABILITY OF DOPED $\delta$ -Bi<sub>2</sub>O<sub>3</sub> AS AN ELECTROLYTE FOR SOLID OXIDE FUEL CELLS

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The high temperature phase of bismuth oxide ( $\delta$ -Bi<sub>2</sub>O<sub>3</sub>) is a promising material for application as an electrolyte for solid oxide fuel cells (SOFCs), due to its high oxygen ion conductivity. Doping with rare earth cations stabilizes  $\delta$ -Bi<sub>2</sub>O<sub>3</sub> phase down to room temperature. According to literature [1], the ionic conductivity of such  $\delta$ -Bi<sub>2</sub>O<sub>3</sub> is not significantly decreased even at 600 °C. This opens the possibility to lower SOFC operating temperature from 1000 °C to intermediate temperatures. The main drawbacks of this material are the instability in reducing atmosphere and reactivity toward electrode materials. Bismuth ruthenate (Bi<sub>2</sub>Ru<sub>2</sub>O<sub>7</sub>) was chosen as a potential electrode material because of its chemical stability, compatibility with  $\delta$ -Bi<sub>2</sub>O<sub>3</sub> and metal-like electronic conductivity.

Stoichiometric mixtures of Bi<sub>2</sub>O<sub>3</sub> with Tm<sub>2</sub>O<sub>3</sub> or Lu<sub>2</sub>O<sub>3</sub> were dry homogenized and heat treated at 750 °C for 3 h in order to obtain  $\delta$ -Bi<sub>2</sub>O<sub>3</sub> with following compositions: (Bi<sub>0.8</sub>Tm<sub>0.2</sub>)<sub>2</sub>O<sub>3</sub> and (Bi<sub>0.75</sub>Lu<sub>0.25</sub>)<sub>2</sub>O<sub>3</sub>, respectively. Bi<sub>2</sub>Ru<sub>2</sub>O<sub>7</sub> was synthesized similarly, i.e. homogenized mixture of Bi<sub>2</sub>O<sub>3</sub> and RuO<sub>2</sub>·xH<sub>2</sub>O was heated at 900 °C for 3 h. The obtained powders were pressed into disc-shaped pellets and sintered at 920 °C in case of  $\delta$ -Bi<sub>2</sub>O<sub>3</sub> and 880 °C in case of Bi<sub>2</sub>Ru<sub>2</sub>O<sub>7</sub>. Chemical stability of these materials was investigated by exposing the pellets to the hydrogen and butane atmospheres. Compatibility of electrode and electrolyte materials was tested by heating a homogenized mixture of Bi<sub>2</sub>Ru<sub>2</sub>O<sub>7</sub> and (Bi<sub>0.8</sub>Tm<sub>0.2</sub>)<sub>2</sub>O<sub>3</sub> (mass ratio 50:50) at 600 °C. Moreover, a mixture of (Bi<sub>0.75</sub>Lu<sub>0.25</sub>)<sub>2</sub>O<sub>3</sub> and Bi<sub>2</sub>Ru<sub>2</sub>O<sub>7</sub> (mass ratio 30:70) was pressed into pellet, sintered at 880 °C, and exposed to hydrogen atmosphere in order to evaluate chemical stability of the mixture under reducing conditions. Both electrolyte- and electrode-supported configurations were considered with the aim to form a functional fuel cell.

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## **NANOCRYSTALLINE SnO<sub>2</sub>-Zn<sub>2</sub>SnO<sub>4</sub> COMPOSITE THICK FILMS APPLIED AS HUMIDITY SENSORS**

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Starting ZnO and SnO<sub>2</sub> nanopowders (<100 nm) were mixed in a suitable ratio and calcined at 1050 °C for 2 hours to obtain nanocrystalline SnO<sub>2</sub>-Zn<sub>2</sub>SnO<sub>4</sub> composite powder. Structural characterization performed by X-ray diffraction (XRD) and Scanning Electron Microscopy (SEM) showed that a nanocrystalline composite SnO<sub>2</sub>-Zn<sub>2</sub>SnO<sub>4</sub> powder was obtained. Thick film paste was made by adding organic vehicles to the powder. Screen printing of four and five layers of thick film paste was performed on two interdigitated test electrode configurations. They were calcined at 500 and 600 °C for 30 minutes. Impedance response was analyzed at several working temperatures (20-60 °C) in the relative humidity range 30-90% and frequency 42 Hz to 1 MHz. Increase in relative humidity lead to a decrease in impedance, especially at lower frequencies. The sensor time delay between absorption and desorption processes was low and the response and recovery times fast showing that the nanocrystalline SnO<sub>2</sub>-Zn<sub>2</sub>SnO<sub>4</sub> composite has potential for application in humidity sensing.

P-15

## THE SOLID SOLUTIONS OF DOPED CERIA PREPARED BY SELF-PROPAGATING ROOM TEMPERATURE METHOD

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A series of doped cerium oxide samples was prepared by simple self-propagating room temperature method (SPRT). The method is known to assure very precise stoichiometry of the final product in comparison with tailored composition. Ceria was doped with various of elements: Co, Mg, Ca, Ba, Mn, Zn, Sr. Dopants were added in 5 and 10% for all of them to obtain a solid solution with composition  $\text{Ce}_{1-x}\text{Me}_x\text{O}_{2-\delta}$  ( $x = 0.05$  and  $0.10$ , whereas Me stands for the dopant element). Results showed that all obtained powders were solid solutions with a fluorite-type crystal structure and all powder particles were nanometric in size. The Raman scattering spectra revealed the existence of  $\text{CeO}_2$  fluorite cubic structure for all investigated samples. The main  $F2g$  mode is shifted to lower energies and is broader than in the spectra of pure ceria doped samples. Red shift and broadening of the  $F2g$  mode can be ascribed to the size and strain effects. The Raman active mode at about  $600\text{ cm}^{-1}$ , seen in all samples, can be ascribed to the  $\text{CeO}_2$  intrinsic oxygen vacancies. Morphology of the samples was observed by FE SRM (field emission scanning electron microscopy).

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## **SYNTHESIS AND APPLICATION OF SILICA PARTICLES FOR THE REMOVAL OF HEAVY METALS AND PESTICIDE RESIDUES FROM AQUEOUS SOLUTIONS**

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In this study, the adsorption behavior of silica adsorbents with different morphology and porosity has been examined in order to evaluate their use for the purification of wastewaters containing toxic environmental chemicals such as heavy metals and pesticide residues. Three different types of silica particles were investigated: (i) microporous silica core particles prepared by the hydrolysis and condensation of tetraethylorthosilicate (TEOS), (ii) mesoporous silica particles generated by the neutralization of highly basic sodium silicate solution and (iii) silica core-shell particles composed of mesoporous silica layers around dense cores. Monodispersed spherical silica particles produced from TEOS have a microporous structure but the lowest adsorption efficiency and adsorption capacity of both heavy metals and pesticides. Polydispersed silica particles of irregular shape prepared from highly basic sodium silicate solution exhibit a mesoporous structure and high efficiency for the removal of heavy metals and pesticides from aqueous solutions. Monodispersed core-shell particles composed of a microporous core and a mesoporous shell also have high adsorption efficiencies in both combinations. Moreover, silica particles can be easily functionalized with ferrite nanoparticles, which allow the magnetic separation of silica adsorbents from aqueous solutions.

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## **TITANIA AND CHEMICALLY MODIFIED TITANIA IN PHOTOCATALYTIC CONVERSION OF SELECTED DYE(S) AND PESTICIDE**

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TiO<sub>2</sub> is one of the most widely investigated and used photocatalysts in water contamination treatments. In order to synthesize TiO<sub>2</sub> and chemically modified titania catalysts with the appropriate characteristics, numerous methods can be applied. One of titania potential application in different waste water treatments is usage in degradation of various organic pollutants harmful to the environment and/or water organisms.

In this work, TiO<sub>2</sub>-based (pure and chemically modified) catalysts were prepared by improved sol-gel procedure by using titanium-isopropoxide as a precursor, and tested in photocatalytic conversion/decomposition of selected pollutants (dye(s) and pesticide). Characterizations of the prepared TiO<sub>2</sub>-based samples were performed by using BET, FE-SEM, XRD method(s)/techniques. Different relatively mild process conditions such as: catalysts dosages, low UV irradiation energy, initial pollutants concentrations, reusability of catalysts (*i.e.* catalyst efficiency under long-run working conditions) were studied in order to optimize the photocatalytic processes.

The obtained results have shown that physico-chemical properties of the pure titania were influenced by chemical modification with modifier. Modified-titania-based catalysts have presented significantly higher photocatalytic efficiency in conversion of selected organic pollutants. The achieved multimodal distribution of pore sizes (PSD), higher amount of mesopores, the presence of mixed crystal phases and improved crystalline structure as well as higher total surface acidity in the case of modified-titania catalysts can be closely related to more effective photocatalytic activity compared to the pure titania catalyst.

Photocatalytic conversion of pesticide was observed with use of hydrogen peroxide in different concentrations in order to optimize the process. It can be noted that decomposition/conversion process was enhanced when H<sub>2</sub>O<sub>2</sub> was used (in so-called Advanced Oxidation Process) compared to the process without hydrogen peroxide.

The photocatalytic performance of pure titania and chemically modified-titania catalysts is strongly influenced by the physico-chemical properties of the synthesized materials. It can be pointed out that suitable porosity (specific surface

area, mean pore diameter, pore volume and PSD), the presence of catalytically active mixed crystal phases and appropriate morphology provided efficient photocatalytic activity, especially when chemically modified catalyst was used.

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P-18

### **PHASE TRANSITION FROM TiO<sub>2</sub> BROOKITE-BASED NANOPOWDER TO TITANATE: EFFECT OF ANNEALING TEMPERATURE ON MORPHOLOGY AND PHOTOCATALYTIC BEHAVIOR**

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TiO<sub>2</sub> nanopowder based on brookite phase was synthesized using sol-gel hydrothermal method, with TiCl used as a precursor [1]. For the purposes of preparing one-dimensional (1D) nanoribbons, the obtained TiO<sub>2</sub> nanopowder was used as a precursor following an alkaline hydrothermal approach [2, 3], after which an annealing process took place. The structural properties of the synthesized nanomaterials were analyzed by X-ray powder diffraction (XRPD). Besides the XRPD pattern, the structural and morphological characteristics of obtained nanopowder and nanoribbon were also investigated by Raman spectroscopy and Field Emission Scanning Electron Microscopy (FESEM). Synthesized nanostructures were tested in photocatalytic degradation of Reactive Orange (RO16) azo-dye, since these dyes represent the most toxic ones among various types of dyes. The TiO<sub>2</sub> brookite-based nanopowder showed the best photocatalytic efficiency, whereas the titanate after annealing were much faster in degradation in comparison with titanate obtained after hydrothermal process.

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P-19

## THE EFFECTS OF MILLING MEDIA ON MORPHOLOGICAL AND STRUCTURAL CHANGES IN MECHANICALLY ACTIVATED ZnO

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Mechanical activation (MA), as a simple and low-cost method for modifying physico-chemical properties of disperse systems, is often used for obtaining powders. Prolonged milling in high-energy mills, necessary for obtaining nanoparticles, leads to contamination of the starting material, and it can be used as an additional route for introducing the milling assembly material as the desired dopant into a powder.

In the present work morphological and structural characteristics of ZnO nano-powders obtained by MA in a high-energy planetary ball mill with stainless steel (Fe), Y-stabilized zirconium oxide (Zr) and tungsten carbide (W) vials and balls were investigated. Knowing that microstructural characteristics of mechanically milled ZnO powder have strongly depended on milling conditions. The milling has been performed in a continual regime in air, with following conditions: the rotation speed of the disk was 400 rpm, ball-to-powder mass ratio was 40:1, and milling time was 300 min. The samples were characterized by scanning electron microscopy (SEM), equipped with an EDS, X-ray diffraction (XRD), Raman and UV-vis spectroscopy. In order to investigate the type of intrinsic defects and impurities introduced by milling, both milled and thermally treated milled ZnO were analyzed.

According to the SEM, the particles of various sizes (100–500 nm) were present in the sample before milling. After milling significant changes in particle shapes and sizes and very pronounced tendency to adhesion in agglomerates, with dimensions in the range of submicron up to a few micrometers, has been noticed.

The phase analysis of both milled and thermally treated milled samples of powders indicates the presence of wurtzite ZnO refined in  $P6_3mc$  space group [1]. The XRD patterns of milled samples of Fe-, W- and Zr-doped ZnO do not reveal the presence of other ZnO phases. On other side, in thermally treated milled samples of W- and Fe-doped ZnO the  $ZnWO_4$  (samartinite,  $P2_1/c$ ) and cubic spinel ( $Fd-3m$ ) are present, respectively. In thermally treated milled Zr-doped sample monoclinic and tetragonal  $ZrO_2$  ( $P2_1/c$  and  $P4_2/nmc$ ) are present, whereas  $ZnZrO_3$  structures could not be refined due to very low peak intensities [2].

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P-20

## FORMATION OF MgO/Mg(OH)<sub>2</sub> NANOSTRUCTURES BY MOLTEN SALT ELECTROLYSIS

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Thanking its unique characteristics, magnesium oxide and magnesium hydroxide nanostructures are of high practical significance for possible application in the next generation of solar cells, electronic devices, displays, in detection and adsorption of different environmental pollutants [1]. Numerous methods of synthesis including precipitation, solvothermal and hydrothermal processes, the sono-chemical technique, the sol-gel method, microwave methods, chemical vapor deposition, carbonatization and electrochemical method are widely used for synthesis of various forms magnesium oxide/magnesium hydroxide nanostructures such as whiskers, platelets, rods, needle-like, flower like etc. Electrochemical method attracts a special attention in a production of nanostructures owing to easy control of morphology of particles by the choice of regimes and parameters of electrolysis.

In this study, the processes of electrolysis from magnesium nitrate hexahydrate melt in the both potentiostatic and galvanostatic conditions were analyzed. Morphologies of synthesized particles were characterized by scanning electron microscopy (SEM) technique. The X-ray diffraction (XRD) analysis of produced particles showed that the mixture of magnesium oxide and magnesium hydroxide was formed by these molten salt electrolysis processes [2,3].

No any difference in surface morphology was observed between these two constant regimes of electrolysis. The very thin needles often grouped in flower-like aggregates were obtained by the electrolysis processes. The special attention was devoted to the effect of hydrogen as parallel reaction to processes of electrolysis. In the dependence of parameters of electrolysis (potential or current density applied), holes formed from detached hydrogen bubbles of various shape and size from dish-like holes to those creating the honeycomb-like structures were formed. Mechanism of formation of all observed morphological forms was considered. Also, comparison with electrolysis processes from aqueous magnesium salt electrolytes was made and discussed.

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3. N.M. Vukićević, V.S. Cvetković, N.D. Nikolić, G. Branković, T.S. Barudžija, J.N. Jovićević, *J. Serb. Chem. Soc.*, **83** (2018) 1351

P-21

## GRAIN MORPHOLOGY OF LOW TEMPERATURE TREATED HYDROXYAPATITE MATERIAL

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Thermal treatment of hydroxyapatite (HAp) material is very important since it provides the final microstructural design and chemical composition, and directly governs the mechanical properties as well as the biological behaviour [1]. Densification of HAp compacts normally require sintering at 1000 °C or higher [2,3]. However, very low temperatures (300–500 °C) are used to preserve the morphology of initial particles and develop microstructures made by nanosized grains [1]. The solution-precipitation method was used for preparing hydroxyapatite material. Synthesized material was thermally treated at 300 °C with different retention time for 3 and 6 hours in air atmosphere. XRPD and SEM analysis were used to investigate phase composition, structural arrangement and grain morphology. Results show that different retention time has influence on grain growth and structural arrangement of hydroxyapatite material. The crystallite size and microstrain parameters were also examined.

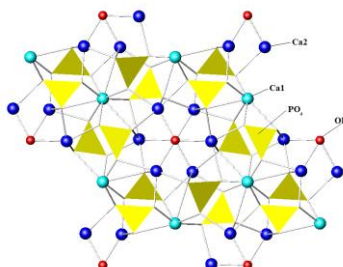


Figure 1. Structure of hydroxyapatite

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P-22

## **CHARACTERIZATION OF SiO<sub>2</sub> CERAMIC POWDER SYNTHESIZED BY INCORPORATION OF A PORE GENERATOR INTO THE ACTIVATED CARBON**

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This research presents obtainment of a carbon solid residue by carbonization process of biomass (from plane tree fruit) in an inert atmosphere, physical activation and chemical treatment (by TEOS - tetraethyl orthosilicate) of carbon that resulted in formation of highly porous and spatially distinct ordered ceramic powder. High-temperature conversion via natural grown system as bulk template led to the creation of ceramics. Carbonization process at high temperature range and 3-cycle activation of carbons with TEOS showed the possibility of synthesizing SiO<sub>2</sub> structures. Fourier-transform infrared (FTIR) spectroscopy has been used for identification of surface-active reaction groups in the ceramic structures. In order to perform qualitative analysis of polytypes, Raman spectroscopy was used. X-ray diffraction (XRD) revealed structural and compositional changes in synthesized porous ceramic powders. Porous morphology of obtained ceramics has been investigated and confirmed by field emission scanning electron microscopy (FESEM) It has been established that porous ceramics can be produced using the described technology during thermal reactions at 600 °C for 1 h, where obtained ceramic materials retain a tubular and honeycomb pore structure of plane tree fruits.

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## FUNCTIONAL PROPERTIES OF SiC-GRAPHENE COMPOSITES AND ITS BASIC EDM CHARACTERISTICS

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Almost fully dense silicon carbide composites with Y<sub>2</sub>O<sub>3</sub> and Al<sub>2</sub>O<sub>3</sub> as a sintering additives and with different amount of graphene nanoplatelets (GNPs) from 5 to 15 wt.% or 5 wt.% of graphene oxide (GO) were sintered in rapid hot press (RHP) at 1800 °C for 5 min with a pressure of 50 MPa in vacuum.

Functional properties (electrical conductivity, thermal diffusivity) of SiC-graphene composites were investigated as a function of GNPs and GO additions and orientations of the graphene layers. Basic electro-discharge machining (EDM) characteristics (material removal rate and surface roughness) were investigated as well.

Composites microstructure anisotropy caused by graphene alignment as a consequence of rapid hot pressing was confirmed by measuring of electrical conductivity and thermal diffusivity. Electrical conductivity increased significantly with increased weight fraction of graphene in both measured directions. Highest value of 2031 S/m was obtained for composites with 15 wt. % of GNPs in parallel direction and only 1246 S/m in perpendicular direction to aligned GNPs. Thermal diffusivity is 63.3 mm<sup>2</sup>/s in parallel and only 23.3 mm<sup>2</sup>/s in perpendicular direction. Material removal rate (MRR) of all SiC/GNPs and SiC/GO composites was higher than 1.6 mm<sup>3</sup>/min during the WEDM tests. MRR was almost doubled and increased to 2.8 mm<sup>3</sup>/min in composite containing 15 wt.% of GNPs. At the same time surface roughness decrease to 1.5 µm.

*Acknowledgement:* This work was supported by the Slovak Research and Development Agency under the contract no. APVV-SK-SRB-18-0022. The support of the MVTs project of SAS “UltraCom” within the scheme of “Seal of Excellence projects” is also acknowledged.

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## **PREPARATION OF Co<sub>3</sub>O<sub>4</sub> NANO- AND MICROPARTICLES BY SOLID STATE THERMOLYSIS OF COBALT(II) COMPLEX**

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Development of nanomaterials such as transition metal oxides with spinel structure has been intensively examined because of their applications in catalysis, energy storage, magnetic data storage and sensors [1]. Synthesis of these materials has been realized by various approaches, such as hydrothermal synthesis, solid state reactions and microwave synthesis [1]. In previous years, thermolysis of transition metal complexes as precursors provides a new technique in preparing useful nanomaterials due to the possibility to control their particle size and morphology [2].

The nano- and microparticles of Co<sub>3</sub>O<sub>4</sub> have been prepared by direct calcination of ternary Co(II) complex, [Co<sub>3</sub>(bipym)<sub>3</sub>(H<sub>3</sub>mell)<sub>2</sub>·18H<sub>2</sub>O, where bipym is 2,2'-bipyrimidine and H<sub>3</sub>mell<sup>3-</sup> is anion of 1,2,3,4,5,6-benzenehexacarboxylic (mellitic) acid at 450 and 1000 °C in air atmosphere. The powder X-ray diffraction (XRD) and scanning electron microscopy (SEM) were used to investigate structure and morphology of the obtained materials. The results indicated the formation of pure Co<sub>3</sub>O<sub>4</sub> phase, whose particles size depends on the calcination temperature.

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## **OPTICAL AND STRUCTURAL INVESTIGATION OF Cr<sub>2</sub>O<sub>3</sub> THIN FILMS: THE EFFECT OF THICKNESS FOR POSSIBLE APPLICATION FOR DIFFERENTIAL PHOTODETECTORS**

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We report experimental study of Cr<sub>2</sub>O<sub>3</sub> thin films (60, 300, 350 nm) deposited on silicone and glass substrate using Balzers Sputtron II System. The structural and optical properties are investigated by means of AFM, XRD, UV-VIS, Raman and infrared spectroscopy, in order to determine suitability of as-obtained films as potential active layers in novel differential inorganic photodetectors. AFM measurements reveal that the films are well-deposited, without presence of any cracks and voids. The wide structures on XRD spectra indicate that the degree of crystallinity in our films is low. UV-VIS measurements reveal strong red shift of absorption maxima with reducing the film thickness. IR and Raman spectroscopy show dependence of characteristic vibrations on film thickness but also on substrate. Our results indicate the Cr<sub>2</sub>O<sub>3</sub> film of 300 nm thickness is the best candidate for photoactive semiconducting layer in differential photodetectors.

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## **PHOTOCATALYTIC ACTIVITY OF BiFeO<sub>3</sub>-BASED POWDERS**

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Bismuth-ferrite (BiFeO<sub>3</sub>) is studied a lot in recent years due to its specific multiferroic properties. Thanks to the optical bandgap energy of 2.3-2.8 eV [1], BiFeO<sub>3</sub>-based materials are also interesting for photocatalytic and solar energy applications. Sol-gel methods were used to produce BiFeO<sub>3</sub> and BiFeO<sub>3</sub>-modified

diatomaceous earth. These powders were characterized, and their visible light photocatalytic activity for decomposition of some organic dyes was tested in acidic, close-to-neutral and alkaline conditions. Fenton-like catalysis was also tested for those materials. Influence of synthesis method, microstructure, ageing and composition on dye degradation helped in proposing the mechanism of adsorption and photocatalytic processes.

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P-27

## **NANOCRYSTALLINE IRON-MANGANITE (FeMnO<sub>3</sub>) APPLIED FOR HUMIDITY SENSING**

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Nanocrystalline iron manganite was synthesized using a sol-gel self-combustion method with glycine as fuel, followed by calcination at 900 °C for 8 hours. Structural characterization was performed using X-ray diffraction (XRD) and field emission scanning electron microscopy (FESEM). It confirmed the formation of nanocrystalline iron-manganite with a perovskite structure. Humidity sensing properties of bulk and thick film samples of the obtained nanocrystalline iron manganite powder were analyzed. Organic vehicles were added to the powder to form a thick film paste that was screen printed on alumina substrate with test PdAg interdigitated electrodes. Impedance response of bulk and thick film samples was analyzed in a humidity chamber in the relative humidity range 30-90% in the frequency range 42 Hz to 1 MHz in view of applying iron-manganite for humidity sensing applications.



P-28

## **STRUCTURAL, OPTICAL AND PHOTOCATALYTIC PROPERTIES OF BiFeO<sub>3</sub> NANOPARTICLES**

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BiFeO<sub>3</sub> (BFO) precursor powder was synthesized by ultrasound assisted sol-gel route at relatively low temperature, starting from Bi-nitrate, Fe-nitrate, and ethylene glycol. Structural, optical, and photocatalytic properties of the obtained powder were investigated. X-ray diffraction analysis confirmed that thermal treatment of precursor powder at 500 °C led to formation of pure phase BiFeO<sub>3</sub>. BFO is p-type semiconductor where determined band gap was 2.20 eV, indicating its potential application as visible-light-response photocatalyst. Mott-Schottky measurements were performed to determine flat band potential and position of valence and conduction bands. Obtained BFO powder is used for photocatalytic degradation of typical organic azo dye Mordant Blue 9 in concentration of 50 mg/l. Measurements were performed for different times of irradiation and pH of the dye solution. Photodegradation products were analyzed by HPLC technique, and mechanism of photocatalytic degradation of organic dye was proposed.

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## **RADIOLOGICAL AND STRUCTURAL CHARACTERIZATION OF FLY ASH-BASED ALKALI ACTIVATED MATERIALS**

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Fly ashes, obtained as waste products, from different sources (wood and lignite) were used as a basic ingredient of the new geopolymeric materials [1]. Presented study deals with the final structure and radiological properties of fly ash-based geopolymers. The technology of geopolymerisation is gaining commercial interest because it has been demonstrated that, in certain cases, the properties of geopolymeric materials are superior to existing cementations systems [2].

Coal fly-ash (CFA) (lignites Kolubara) and wood fly ash (WFA) were obtained in combustion process. Synthesis of the geopolymers was conducted by mixing fly ash, sodium silicate solution, NaOH and water. The samples were cured at 60°C for 48h after staying at room temperature in covering mold for 24<sup>h</sup>. XRD, FTIR and SEM-EDS measurements of the samples after 28 days process of geopolymerization were done. X-ray diffraction measurements of CFA samples show anhydrite as the main constituent, while WFA samples consist of calcite, albite and gypsum minerals. The largest part of the geopolymers structure is amorphous and glass-like. Fourier transform infra-red (FTIR) and SEM-EDS analysis were applied for determination a polymeric Si–O–Al framework and microstructure of investigated samples, respectively.

Beside of determination of physical-chemical properties, the aim of this study was radiological characterization of CFAs, WFAs and the obtained geopolymer products. Activity concentration of <sup>40</sup>K and radionuclides from the <sup>238</sup>U and <sup>232</sup>Th decay series in ash samples and fly ash-based geopolymers were determined by means of gamma ray spectrometry, and the absorbed dose rate (D) and the annual effective dose rate (E) were calculated in accordance with the UNSCEAR 2000 report.

**Keywords:** CFA, WFA, Geopolymerization, XRD, Radionuclides

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P-30

## **ELECTROCHEMICAL SENSORS BASED ON PYROPHYLLITE**

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Pyrophyllite is a phyllosilicate mineral composed of aluminium silicate hydroxide:  $\text{Al}_2\text{Si}_4\text{O}_{10}(\text{OH})_2$ . Due to excellent physicochemical characteristics, such as low thermal and electrical conductivity, low expansion coefficient, low reversible thermal expansion and excellent reheating stability, it is widely used in many industries. The aim of this study is to examine the pyrophyllite for its potential application for electrochemical sensors. Mechanochemical modification using SPEX Mixer/Mill 5100 was used to generate desired products with fine structures. The structural changes of pyrophyllite before and after the milling process have been investigated by means of PSD (particle size distribution), XRD (X-ray diffraction), FTIR (Fourier-transform infrared spectroscopy) and DTA-TG (differential thermal analysis-thermogravimetric analysis). Pyrophyllite carbon paste electrode based on tricresyl phosphate as a binding liquid has been applied as working electrode for the voltammetric characterization and determination of the carbendazim fungicide [1]. It is demonstrated that the carbon paste electrode modified with pyrophyllite can be used like electrochemical sensors for pesticides.

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P-31

## **METAL-GLASS COMPOSITE MATERIAL**

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The aim of the paper is to create a metal-glass composite material as well as to examine the possibility of using this composite material for industrial application. Powder of commercial austenitic stainless steel (SURFIT TM 316L) of the diameter from 45 to 63 µm was used in this the experiment. The steel powder of the spherical shape is obtained by atomization of gas. The source of glass was basalt rock from the locality "Vrelo" Kopaonik, Republic of Serbia, due to relative low melting point and low viscosity. Composite materials were manufactured by mechanical mixing steel powders with fresh crushed basalt rock in diameter below 45 µm. Mixtures of basalt content of 10, 30 and 50 wt.% were prepared.

Green compacts were obtained by pressing under pressure of 150 MPa using a steel mold. Thermal treatment is done at 1250 °C for 30, 45 and 60 minutes in a vacuum furnace. Starting powder as well as sintered composites were characterized by X-ray diffraction method (XRD). Morphology of powders and microstructural development were followed by scanning electron microscope (SEM). Mechanical properties were investigated by Vickers hardness.

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## **MICROSTRUCTURAL ANALYSIS AND MICROHARDNESS OF IRON DOPED MULLITES**

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The analysis of microstructure and microhardness of sintered iron doped mullite samples has been preformed after synthesis, heat treatment and sintering of the chemically synthesized iron doped mullite precursors. The iron doped mullite precursor powders were synthesized by sol-gel combustion method with 3:2 mullite compositions up to 15 wt.% of Fe<sub>2</sub>O<sub>3</sub>. After the synthesis and additional heat treatment at 800 °C, the mullite precursor powders were coarse and consisted of the coalesced particles. During the combustion and heat treatment at 800 °C, added iron was likely to lower the temperature of early forming of liquid phase that filled the pores between powder particles. This early-formed liquid phase enhances higher velocities of diffusing species and consequently growth of powder particles. Despite the appearance of “hard” agglomerates, that could impede the material densification, high microhardness values are achieved. Depending upon the iron content, the microstructure of sintered samples altered in terms of shape and size of the developed grains. The low-iron mullite precursors developed the needle-like grain morphology like undoped mullite, whereas the high-iron mullite precursors, above 9 wt.% of Fe<sub>2</sub>O<sub>3</sub>, evolved the rod-like or lath-like mullite grains. Even though, the obtained density values were not high, the measured values of Vickers hardness (HV0.1) were satisfying due to the characteristic mullite microstructure regarding the stiff skeleton of intertwined mullite grains.

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## PHASE COMPOSTION AND SYNTERING BEHAVIOR OF BORON SUBOXIDE (B<sub>6</sub>O) CERAMICS

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Boron-rich phases have good physical and chemical properties, such as high hardness, low mass density, high thermal conductivity, high chemical inertness and excellent wear resistance [1,2]. Properties of B<sub>6</sub>O suggest that it can be a good candidate to be used in the manufacturing of abrasives, cutting tools and scratch-resistant coatings.

B<sub>6</sub>O powders were produced at the reaction temperatures between 1200 and 1500 °C for 1 hour without pressure. The structure and properties of samples were characterized by X-ray diffraction and scanning electron microscopy field emission. XRD analysis showed that the purity of the powders increases with reaction temperature with corresponding increase in the crystallite size. SEM image obtained at higher temperature clearly showed improved crystallinity as the reaction temperature was increased. B<sub>6</sub>O powder prepared at 1500 °C exhibited an oxidation resistance in air up to 600 °C and mild oxidation in temperature range of 700–1000 °C. B<sub>6</sub>O powders were then sintered at higher temperatures via hot-press. According to analysis, samples contain second phase B<sub>4</sub>C at 1800 °C and have Vickers hardness of 20 GPa, due to the porosity.

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## IS THERMOSALIENT EFFECT POSSIBLE WITHOUT PHASE TRANSITION?

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Oxitropium bromide and methylscopolamine bromide have very similar molecular structures, the only difference being that one ethyl group is replaced by methyl group in the case of methylscopolamine bromide. Both compounds have medical uses, oxitropium bromide is used as a bronchodilator, whereas methylscopolamine bromide used to prevent nausea and vomiting caused by motion sickness. They also both exhibit thermosalient effect – unexpected and abrupt jumping of the crystals during heating and cooling. This is where the difference stops. In the case of oxitropium bromide thermosalient effect is caused, as in most other thermosalient compounds, by the topotactic phase transition during which unit cell changes drastically thus causing the crystals to jump to heights several times larger than their dimensions. At the molecular level, the cation acts as a molecular shuttle composed of two rigid parts (epoxy-aza-tricyclic-nonyl portion and phenyl ring) that are bridged by a flexible ester linkage. The structure of the rigid, inert aza-tricyclic portion remains practically unaffected by the temperature, suggesting a mechanism in which the large, thermally accumulated strain is transferred over the ester bridge to the phenyl ring, which rotates to trigger the phase transition [1].

On the other hand, surprisingly, methylscopolamine bromide does not seem to show any phase transition at all, but yet, its crystals are also joyfully jumping around during the heating or cooling of sample.

Both systems are characterized by uniaxial negative thermal expansion, but there is an abrupt change of the unit cell parameters during the phase transition for the oxitropium bromide whereas the parameters are changing perfectly linearly in the whole temperature range of existence for methylscopolamine bromide. Therefore, the question remains - what is causing the jumping in methylscopolamine bromide - a system so close to oxitropium bromide but exhibiting totally different kind of thermosalient effect.

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## CRYSTAL STRUCTURE PREDICTION IN Y-TERNARY SYSTEMS

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Rare-earth (RE) oxysulfides have many applications such as solar energy, wind turbines, batteries for electric vehicles and mobile phones, cathode ray tubes, metal alloys, ceramic materials and so on. Their important feature is that those materials are wide-gap semiconductors. Yttrium oxide is one of the most important compounds of yttrium and is widely used in many ceramic materials. RE element-doped oxysulfides have been utilized for efficient luminescent use e.g., Eu-activated  $\text{Y}_2\text{O}_3\text{S}$  emits bright red-light under cathode-ray excitation and has been widely used for televisions [1]. In this study, we performed crystal structure prediction and investigate energy landscape of yttrium oxisulfide ( $\text{Y}_2\text{O}_3\text{S}$ ). In order to predict new crystal structures, global optimizations on the energy landscape of  $\text{Y}_2\text{O}_3\text{S}$  have been performed using empirical potentials. Afterwards, a local optimization has been performed using ab initio calculations [2]. In particular various quantum mechanical methods have been applied: Density Functional Theory (DFT) with Local-Density Approximations (LDA) and Generalised Gradient Approximation (GGA), and hybrid B3LYP (Becke, three-parameter, Lee-Yang-Parr) functional. Our calculations were in good agreement with the experimentally observed trigonal structure (space group  $P-3m1$ , no. 164). Furthermore, novel modifications of pure yttrium oxisulfide have been discovered with the change of pressure and/or temperature.

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P-36

## DFT STUDY OF Au / Ag / Cu DOPED TiO<sub>2</sub>

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Titanium dioxide is a widely investigated photocatalytic material with many practical applications. Doping TiO<sub>2</sub> enhanced interactions with biological systems, decontamination of pollutants (water, soil), and conversion of solar energy. Au / Ag / Cu doped TiO<sub>2</sub> particles showed toxic effects on cervical cancer cell lines, and on human colon carcinoma [1]. Adding nanoparticles of silver improves antimicrobial effects of photocatalytic systems, and similarly, the cytotoxic activity of Cu in TiO<sub>2</sub> results in a high bactericidal activity even under very weak UV light [2]. Geometrical optimizations of various bulk modifications have been performed using density functional theory (DFT), with LDA exchange-correlation functional implemented in the CRYSTAL17 code [3]. The optimized titanium dioxide structures have been doped with Au, Ag and Cu cations, creating large supercells to mimic the results of the experiment. The geometrical optimizations of doped TiO<sub>2</sub> have been performed in a similar manner to undoped TiO<sub>2</sub>. The results of the theoretical studies of doped TiO<sub>2</sub> can contribute to the design of better antimicrobial and antitumor agents.

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P-37

## THEORETICAL INVESTIGATION OF VARIOUS TiO<sub>2</sub> MODIFICATIONS AND THEIR ELECTRONIC PROPERTIES

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Titanium dioxide (TiO<sub>2</sub>) is a wide-gap semiconductor that has been widely investigated due to its photocatalytic properties and applicability for various purposes, such as solar cells, decontamination of pollutants, elimination of microorganisms, suppression of cancer cells, etc. Extensive experimental and theoretical studies of TiO<sub>2</sub> can give different data on the stability of individual modifications and their transitions. We performed *ab initio* optimizations of various bulk modifications of TiO<sub>2</sub> using density functional theory (DFT), with LDA and hybrid B3LYP exchange-correlation functional implemented in the CRYSTAL17 code. In order to get insight into the theoretically most stable modifications and potential candidates for further research, energy/volume ( $E(V)$ ) and enthalpy/pressure ( $H(p)$ ) dependence curves have been calculated. Furthermore, electronic properties were calculated and analyzed for each of the investigated TiO<sub>2</sub> phase.

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## STRUCTURE PREDICTION AND ENERGY LANDSCAPE EXPLORATION IN THE CrSiN SYSTEM

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There is a serious need for protection coatings for various machinery, especially equipment operating in harsh conditions such as marine environment. Due to its outstanding properties, CrN is widely used as a protective coating. However, it is not suitable for usage in the extreme conditions due to its high friction coefficient. A number of studies indicate that implementation of Si in the CrN complex can significantly improve its performance. As several studies have shown, CrSiN coating is comprised of two phases, where the nanocrystalline CrN is embedded in Si<sub>3</sub>N<sub>4</sub> amorphous matrix. Within this study, we present the first investigation of the bulk CrSiN max phases, since previous experimental studies report only CrSiN in thin films. In order to get insight into structural stability of the possible phases existing in this system, we have performed global explorations of the energy landscape of the bulk CrSiN using simulated annealing with an empirical potential [1,2]. This was followed by local optimization on *ab initio* level, with calculations performed with density functional theory (DFT) using LDA and GGA functional. As a result, a number of low symmetry structure candidates have been found in the Cr<sub>2</sub>SiN<sub>4</sub> compound. As earlier studies have shown outstanding properties of CrSiN coatings, it is of crucial importance to further investigate this ternary system in order to determine the properties of these newly discovered phases, and possibilities for industrial and technological applications.

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## **SILICON HEXABORIDE INVESTIGATIONS USING *ab initio* DATA MINING APPROACH**

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Silicon borides are light weight ceramics with very wide application due to their outstanding properties. Silicon hexaboride is a very desirable industrial material discovered in 1900, and it is considered to be one of the most enigmatic refractory compound. On the other hand, the crystal structure is yet not fully understood in the literature. The first reports suggested a cubic SiB<sub>6</sub>, which was followed by experimentally observed orthorhombic phase. Later studies determined a cubic SiB<sub>6</sub> as an unstable phase and suggested additional monoclinic *P21/m* space group. In order to investigate suggested phase and predict novel models we have undertaken calculations using *ab initio* minimization data mining approach [1,2]. Unknown structure candidates in the SiB<sub>6</sub> system have been generated using data mining, followed by local optimization. *Ab initio* calculations were carried out on density functional theory (DFT) level using LDA and GGA functional. Additionally, elastic constants and mechanical properties for each of the predicted modification have been investigated. Since the ability to operate in the extreme environments of SiB<sub>6</sub> modifications was considered, it is very important to further explore these newly discovered phases and investigate in detail their properties, in order to find new possibilities for future industrial and technological applications.

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P-40

## **ADAPTATION OF N-TiO<sub>2</sub> PROPERTIES USING TARGETED DEPOSITION OF TRANSITION METALS**

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The ongoing effort to boost the renewable energy in everyday life makes hydrogen as a fuel an increasingly attractive concept. However, before fully integrating the hydrogen economy into energy revolution, hydropower systems still need an upgrade in energy efficiency, safety, and cost reduction. Among other ways, hydrogen is produced via electrolytic water splitting, using an external energy source, such as solar power, to generate the electricity to split water into hydrogen and oxygen. This is environmentally friendly and efficient, but still too expensive for a large-scale sustainable hydrogen production. If the water splitting is carried out using already available solar power, the electrolytic cell can be omitted from the system, thus reducing the number of steps in the manufacturing process. This concept can be economically acceptable if high solar-to-hydrogen efficiency is achieved. With this in focus, a number of research studies address the potential of various materials as future hydrogen generators.

The presented research combines theoretical and experimental scientific methods to address the potential for integration of two separate renewable energy technologies into one sustainable technology. Solar energy based hydrogen production presents a viable milestone in the renewables economy, yet due to lack of understanding of basic processes that can increase its utilization, it is still an incomplete concept. Phenomena of hydrogen dynamics on the surface of the photocatalytic semiconductor are determined by its inherent electronic structure, while the quantum nature of electrons lies within the field of fundamental research. The theoretical modelling and simulation of photochemical processes correlated with hydrogen behaviour on the electronic level predict possible interactions on interfaces of photochemical cells, while the experimental analysis further verifies these predictions. The collaborative scientific effort provides an extensive overview of the novel information, which can be used to guide and accelerate technological progress.

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## INFLUENCE OF Ho DOPING ON STRUCTURAL AND MAGNETIC BEHAVIOUR OF MULTIFERROIC BiFeO<sub>3</sub>

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Magnetoelectric multiferroics, showing simultaneous ferroelectric and ferromagnetic ordering, have aroused wide attention in recent years, because they offer a wide range of potential applications in data storage media, spintronics and multi-state memories. The influence of Ho doping on the crystal structure and magnetic properties of bismuth ferrite (BFO) nanopowders was investigated. BiFeO<sub>3</sub> and Bi<sub>1-x</sub>Ho<sub>x</sub>FeO<sub>3</sub> ultrafine nanopowders were synthesized by the hydrothermal method. Here we use simple, low-cost and energy-saving hydrothermal method, which has advantages over the conventional methods. The diffraction pattern was recorded at room temperature and atmospheric pressure in the absence of any re-heating of the sample. A fitting refinement procedure using the Rietveld method was performed which showed the incorporation of Ho<sup>3+</sup> ions in the BiFeO<sub>3</sub> crystal lattice, where they substitute Bi<sup>3+</sup> ions. All the samples belong to *R3c* space group. In addition, theoretical investigation using bond valence calculations have been performed in order to mimic pure and Ho doped BiFeO<sub>3</sub> compounds produced in the experiment. Various BFO polymorphs were investigated as function of holmium concentration and final optimization of crystal structures has been performed on *ab initio* level using Density Functional Theory (DFT). Magnetic behaviour of synthesized materials was investigated by SQUID magnetometer in wide temperature interval (2–800 K). Splitting between the zero-field-cooled and field-cooled magnetization curves becomes more pronounced as the Ho concentration is increased, pointing to the development of weak ferromagnetic moment, which is usually connected with uncompensated spins or spin canting. Hysteresis loops show the same fact, attaining higher magnetization with more Ho included, and becoming wider, i.e. magnetically harder.

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## THEORETICAL STUDY OF GdMnO<sub>3</sub> PEROVSKITE STRUCTURES AND INVESTIGATION OF RELATED TILT SYSTEMS

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Rare-earth manganite GdMnO<sub>3</sub> with perovskite structure type has been investigated in a significant number of experimental and theoretical publications [1,2] for its unusual magnetoelectric properties. Structure prediction study of GdMnO<sub>3</sub> focusing on structures generated by octahedral tilting according to group–subgroup relations from the ideal perovskite type (*Pm-3m*), which is the aristotype of the experimentally known GdMnO<sub>3</sub> compound in the *Pnma* space group has been performed [3]. Using structure prediction SPuDS software we have proposed new GdMnO<sub>3</sub> candidates with perovskite structure type, which stability was estimated according to the values of Goldschmidt tolerance factor  $G_t$  and global instability index  $G_{II}$ . Further, for the obtained perovskite structure candidates we have performed a local optimization on the *ab initio* in order to find new modifications accessible with different experimental routes. In this purpose we have used three different *ab initio* approaches: density-functional theory (LDA), hybrid B3LYP and the Hartree-Fock.

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## **THEORETICAL AND EXPERIMENTAL STUDY OF POLYCRYSTALLINE PHASES OBTAINED BY THE NANOMETRIC ZnTiO<sub>3</sub> POWDER SINTERING**

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In this study we have combined two research methods: structure prediction of ZnTiO<sub>3</sub> using computational SPuDS software, and the characterization of binary oxides obtained from ZnO TiO<sub>2</sub> system. Pure nanosized ZnTiO<sub>3</sub> (99.5%), was compacted in cylindrical shape specimens by uniaxial double sided compaction and then sintered in air atmosphere in a dilatometric device [1,2]. One compact was sintered up to 915 °C to retain metastable ZnTiO<sub>3</sub> and held 5 minutes on that temperature, and another one at the same conditions, but now up to 970 °C to induce phase transition and to obtain stable Zn<sub>2</sub>TiO<sub>4</sub> and TiO<sub>2</sub> according to phase diagram [2]. Reheated samples obtained at different characteristic temperatures in air were analyzed by X-ray diffraction (XRD). The infrared attenuated total reflectivity measurements confirmed XRD results. In order to estimate theoretical stability of these perovskite structure, Goldschmidt tolerance factor Gt and global instability index GII were calculated. Furthermore, the Ti valence states were determined by bond valence calculations (BVC). Also, we have investigated the formation of new phases (Zn<sub>2</sub>Ti<sub>3</sub>O<sub>8</sub>, TiO<sub>2</sub> and Zn<sub>2</sub>TiO<sub>4</sub>) originating from ZnTiO<sub>3</sub> with temperature change, as well as the relation between the crystal structures which have been predicted and the structure of the phases we have experimentally observed.

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## STRUCTURAL INVESTIGATION OF INVERSION BOUNDARIES IN Sb-DOPED ZnO

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Basal-plane inversion boundaries (b-IBs) are the most common type of planar faults in zinc oxide, causing inversion of polarity. They can be triggered by the addition of specific IB-forming dopants: In<sub>2</sub>O<sub>3</sub>, Fe<sub>2</sub>O<sub>3</sub>, Mn<sub>2</sub>O<sub>3</sub>, SiO<sub>2</sub>, SnO<sub>2</sub>, TiO<sub>2</sub> and Sb<sub>2</sub>O<sub>3</sub>. Depending on the type of dopant they can either display head-to-head ( $\rightarrow | \leftarrow$ ) or tail-to-tail ( $\leftarrow | \rightarrow$ ) configuration.

In this work, we investigated atomic structure of basal-plane head-to-head IBs in Sb-doped ZnO ceramics by high-resolution transmission electron microscopy (HRTEM) and high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM). Using elementary crystallographic operations, five different translational states for IBs were identified, wherein three of them were experimentally observed. [1–3] By using density functional theory (DFT) calculations, the IBs models were structurally optimized and analyzed in terms of stability for Sb-doping. In the examined cases we obtained a good match between the experimental results and the calculated ones for two of the translations.

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P-45

## MICROSCOPIC AND COMPUTATIONAL STUDY OF Gd-DOPED BiFeO<sub>3</sub>

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Bismuth ferrite, BiFeO<sub>3</sub>, is a promising multiferroic material, with both ferroelectric and magnetic order parameters at room temperature. It crystallizes in rhombohedrally distorted perovskite structure (space group *R3c*), with unit cell parameters  $a = 5.5775(5)$  Å and  $c = 13.8616(8)$  Å [1]. Despite the room-temperature multiferroicity, the use of BiFeO<sub>3</sub> in practical devices has been limited regarding a large leakage current induced by point defects, low magnetic moment and a very weak magneto-electric coupling. The addition of small amounts of trivalent rare-earth elements is known to stabilize the BiFeO<sub>3</sub> phase, and improve its multiferroic properties. The addition of La, Sm, Pr, Eu, Dy and Gd [2] resulted in significant enhancement of magnetization. Based on our previous research of Gd-doped BiFeO<sub>3</sub> (Bi<sub>1-x</sub>Gd<sub>x</sub>FeO<sub>3</sub>), some properties exhibited deviation from regular trends and pointed out to possible formation of superstructures. To study the actual ordering of superlattices we have employed the high-resolution transmission electron microscopy (HRTEM) and high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM). Microscopic analysis had confirmed the initial hypothesis of the supercell obtained by Rietveld analysis of XRPD data for Bi<sub>0.9167</sub>Gd<sub>0.0833</sub>FeO<sub>3</sub>. Based on Rietveld refinement, HRTEM and HAADF-STEM, several models of Gd-doped BiFeO<sub>3</sub> supercells were constructed. Density functional theory (DFT) calculations of constructed models were employed to study the stability range of BiFeO<sub>3</sub> superlattices with respect to different Gd positions.

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## **NOVEL APPROACH TO DOPANT TREATMENT IN ELECTRONIC STRUCTURE CALCULATIONS – A CASE STUDY OF Mg-DOPED ZINC OXIDE**

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A commonly used method for modifying a crystal is doping, where a portion of lattice positions occupied by an element in a structure is taken up by another element (dopant). It is therefore important to determine how doping a crystal influences its stability. Zinc oxide is a semiconductor with wide spectrum of potential application – LEDs, gas sensors, battery anodes, and even more when doped – changing its magnetic, electrical or optical properties by doping opens possibility for other applications like in spintronics.

In order to examine the influence of dopant on stability, we have decided to observe magnesium-doped zinc oxide in a computational model. Using isovalent dopant makes the study simpler, and Mg-doped ZnO has been extensively studied in theory and experiment, which makes it a good basis to compare our findings to previous studies. We assumed that periodic dopant placement would contribute to lower energy of the system compared to a random dopant placement, thus we decided to use a supercell model periodically replicated in 3D space. This approach can indicate whether formation of superstructures can be expected in experiment based on enthalpic contribution of the periodically placed dopant. Our model supercell is made of eight unit cells (2×2×2) with one zinc (6.25 at.%) replaced with magnesium. Using linearized augmented planewave (LAPW) method in combination with quantum theory of atoms in molecules (QTAIM), our aim is to determine energy contribution of a zinc atom in the pure zinc oxide structure and that of magnesium replacing zinc in the doped supercell in order to show how doping contributes to stability of the crystal structure. The goal of this combined approach is to go beyond thermodynamics expressed in terms of simple energy differences. Using unique and physically meaningful partition of unit cell space it is possible to calculate various integral contributions (charge density, energy) of dopant embedded at the particular atomic site. The precise electronic structure is determined using methods that extend beyond DFT, like LDA+U Hubbard approach and hybrid functionals for exact description of exchange term in the Hamiltonian of the system.

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## OPTIMIZATION OF THE PREPARATION OF NOVEL POLYMER/CLAY NANOCOMPOSITES

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Recent advances in material technologies have resulted in the preparation of novel polymer/clay composites with improved thermal, mechanical, optoelectronic/magnetic properties and increased biodegradability [1].

In this study, six samples of poly(glycidyl methacrylate-*co*-ethylene glycol dimethacrylate) (PGME) nanocomposites with organically-modified montmorillonite clay Cloisite 30B<sup>®</sup> (C30B), were prepared via suspension copolymerization. In order to obtain nanocomposites with fine spherical beads of regular shape and satisfying thermal stability the optimization of the synthesis conditions was performed. Firstly, the influence of the poly(*N*-vinyl pyrrolidone) (PVP) quantity in the aqueous phase was varied (1, 3 and 5 wt.%) at a constant stirring rate of 250 rpm and constant clay content C30B (10 wt.%). In the second phase of the optimization of the preparation, samples with a constant composition of the composite reaction mixture (5 wt.% PVP and 10 wt.% C30B) at a stirring rate of 250, 325 and 400 rpm, were prepared. According to the obtained results, it was concluded that the optimal conditions for preparation of these composites are 5 wt.% of PVP and 400 rpm.

The prepared nanocomposites were characterized with Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM) and thermogravimetric analysis (TGA) in air. The structure of the prepared nanocomposites was confirmed with FTIR spectroscopy. According to the obtained SEM microphotographs the fine spherical beads, with desired size and homogeneous morphology, were prepared. Furthermore, SEM analysis was also showed that clay nanoparticles are homogeneously dispersed both inside surface and cross-section area. The incorporation of C30B clay increased the thermal stability of the prepared polymer/clay nanocomposites in comparison to the pure PGME copolymer.

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## MULTIFERROIC COMPOSITES

### **BaTiO<sub>3</sub>-Ni<sub>0.7</sub>Zn<sub>0.29</sub>Cu<sub>0.01</sub>Fe<sub>1.95</sub>Sm<sub>0.05</sub>O<sub>4</sub>**

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Multiferroics are a class of multifunctional materials (a single phase or multiphase/composite materials) characterized by the coexistence of at least two ferroic orders (ferroelectric, ferromagnetic, or ferroelastic). Numerous multiferroics are being developed during the years of intensive research. As compounds with good ferroelectric and piezoelectric properties, barium titanate based materials are usually used as a constituent of these composites and nickel ferrite based materials as a constituent with magnetic properties [1].

The nickel ferrite combines wide range of useful magnetic properties with relatively low electrical conductivity and high value of magnetization. In order to improve electrical and magnetic properties of this material it is usually doped with Jahn-Teller ions such as zinc, manganese or copper [1,2].

Composite ceramics prepared by mixing barium titanate (BT) and nickel zinc (NZF) ferrite doped with Cu and Sm in different mass ratios, BT-NZCSF/70-30, BT-NZCSF/80-20 and BT-NZCSF/90-10 were sintered at 1080 °C for 4 h. The formation of barium titanate tetragonal crystal structure and nickel zinc ferrite cubic spinel structure was identified. Polygonal grains of both constituents were homogeneously distributed in the ceramic samples. Ferroelectric hysteresis loops were roundish and not typical for classical ferroelectric material due to high conductivity of ferrite phase in the materials. The composition with the highest concentration of BT possessed the lowest value of leakage current density. Impedance spectroscopy analysis has shown that total resistivity of the BT-NZCSF/70-30 composition is the lowest due to the highest concentration of conductive ferrite phase in the system. Temperature dependence of the grain and grain boundary conductivity was analyzed using the Arrhenius equation. The activation energies were approximately from 0.2 eV up to 0.5 eV, suggesting the mechanism of polaronic conduction of both, *n* and *p* types. When investigated materials were placed in the humid atmosphere, the fastest change in resistivity was noticed in the composite material with the highest concentration of barium titanate.

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## **THE PRODUCTION OF BIOMORPHOUS CERAMICS AND GLASS-CERAMICS**

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Scientists have been working on reconstructing certain physiological functions of a human body with more or less success by implanting non-organic materials into it. Continuously increasing medical knowledge of the human body, new materials and techniques has brought the renaissance of the dental implants in late 1950s. At first these were made from various biocompatible metals and alloys (Ta, Ti, Cr-Co-Mo, etc.) moulded into different shapes and implanted into the places of a missing teeth in the jawbones, although it was a well known fact that for doctors that the body identifies certain metal implants as foreign materials, encapsulates them and sooner or later rejects them. The discovery of the bioceramics gave a new momentum for the research of biocompatible materials in the early 1960s.

Bioceramics can be biologically inert (bioinert) or bioactive. The later one can be divided into two groups: soluble (hydroxyapatite) or surface-active (bioactive glasses and glass ceramics). The most important part of this work is the production of bioactive ceramics and compare them in a certain point of view.

The living organism found in the nature (for example: plants, trees, animal bones) developed an optimal structure against a specific set of mechanical stresses and living conditions. Copying these structures or using them as a bio-template during the production of artificial materials (e.g.: bioceramics, bioactive glass-ceramics) can result improvement of certain properties of these materials.

During this work biomorph ceramic samples were produced in which pre-treated, protein free animal bones (with various bone structures) were used as bio-templates and these were impregnated with ethanol containing slurries of artificial hydroxyapatite ( $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$ ) powder and hydroxyapatite gel. During this study bioactive soluble ceramics were prepared in order to get biomorph ceramics whose have a composition of trace elements similar to human bones and which could be dissolved in body fluids but with different rate than the impregnated materials. These bioceramics may have a higher mechanical strength and tailorable dissolution rate. All the samples were heat-treated at 950 °C, 1000 °C and 1100 °C, were examined and compared their phase composition, morphology, porosity, specific surface and solubility in simulated body fluid in order to select the appropriate material as a possible implant.

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## **PRODUCTION OF CRACK-FREE CATALYST SUPPORTS FROM METAKAOLIN BASED GEOPOLYMERS**

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Geopolymers or alkali activated inorganic polymers (AAIPs) are non-cement based binders. These materials can be synthesized from alumina, silica and CaO rich materials by treating it with alkaline solutions. As starting material we can use natural material for example kaolin, bentonite, trass or industrial waste for example fly ash and ground granulated blast furnace slag. Besides that, AAIPs can be used to replace cement-based traditional binders due to their high strength, these materials can also easily be well foamed. These foams are eco-friendly porous materials, which have favorable production conditions and promising properties (low shrinkage after foaming, mechanical and chemical stability, high temperature resistance, etc.). These materials can be used, inter alia, in photocatalytic degradation processes or as catalyst supports, membrane supports, heavy metal adsorbents. For this purpose, open porosity AAIP foams are required, which can be produced by combined method (gelcasting/saponification/peroxide – GSP). However, the application of the foams with an open porosity up to 70 vol.% is limited because of their low compressive strength (~0.45 MPa) and high cracking tendency. After solving the above mentioned problems these materials can be used as a catalyst support for photocatalytic sewage treatment processes.

The aim of this work was to develop catalyst supports with optimal composition and adequate strength. Metakaolin based geopolymer foams were produced by GSP combined method using sunflower oil as surfactant and H<sub>2</sub>O<sub>2</sub> as foaming agent. Furthermore, the relationship between strength and structure was investigated, using FT-IR, XRD and SEM. The organic matter content disturbed the photocatalytic degradation processes, which can be removed by calcining the specimen with appropriate firing parameters. Although the samples have good compressive strength, visible hairline cracks appear on their surface and also microcracks inside of them. Results show that change in curing temperature and treatment time have critical influence on the cracking tendency, especially in the early-stage of geopolymerization reaction. The produced crack-free foams can be used either alone or as catalyst supports in photochemical decomposition processes.

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## **PROMISING DENTAL MATERIALS BASED ON $\alpha$ -TRICALCIUM PHOSPHATE AND FLUORAPATITE**

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A new trend in the treatment of tooth is the application of material that would fill the cavity after removal of damaged dental tissue and also remineralize the surrounding tissue. The appropriate material could be a composite of  $\alpha$ -tricalcium phosphate ( $\alpha$ -TCP) and fluorapatite (FAP). The advantage of this material is possibility of  $\alpha$ -TCP to transform spontaneously into hydroxyapatite (HAP) after application, which together with FAP makes the biomaterial very similar to the dentine of the teeth.

The powders of FAP and HAP have been prepared by hydrothermal method, whereas the  $\alpha$ -TCP has been obtained by calcination of HAP at 1500 °C for 2 h. All powders were analyzed by Fourier transform infrared spectroscopy (FTIR), field emission scanning electron microscopy (FESEM), powder X-ray diffraction analysis (XRDP), and energy-dispersive X-ray spectroscopy (EDS). XRDP analysis showed the phase purity and high crystallinity of powders, while FESEM analysis of FAP revealed his rod-like particles morphology and average particle size of 80 nm.

The pills (5×5×5 mm) were made from the mixture of  $\alpha$ -TCP and FAP (wt.% of FAP: 0, 2.5, 5.0, 7.5, and 10.0), using 2.5 wt.% solution of Na<sub>2</sub>HPO<sub>4</sub>. Then, the pills were kept in the simulated body fluid for 3, 10, and 30 days. After this period, mechanical testing of pills was performed, showing that they have satisfactory mechanical properties compared to pills without FAP. Analysis of microstructure with FESEM revealed that on the surface of the pills a new layer of HAP from SBF was formed, confirming good bioactive properties of this material.



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**REMOVAL OF Pb<sup>2+</sup> AND Cd<sup>2+</sup> FROM AQUEOUS SOLUTION  
USING AMINO FUNCTIONALIZED THREE-DIMENSIONALLY  
ORDERED (3DOM) ALUMINA**

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The adsorption of alumina, doped with iron oxide and modified with (3-aminopropyl)triethoxysilane (APTES), FeAl<sub>2</sub>O<sub>3</sub>APTES, was investigated for Pb<sup>2+</sup> and Cd<sup>2+</sup> removal. The structural and surface/textural properties were characterized by FT-IR spectroscopy, TG, XRD, BET and point of zero charge determination. Parameters, such as contact time, adsorbent dosage and temperatures, were examined in the batch conditions. Concentrations of the examined cations, before and after adsorption experiments, were determined by using Atomic Absorption Spectroscopy (AAS). For determination of the adsorption capacities, the best fit was obtained using Freundlich model of the adsorption isotherm.

*Acknowledgments:* This study was financially supported by the Serbian Ministry of Education, Science, and Technological Development (Project No. 176018 and Project No. 172013).

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## **MESOPOROUS SILICA-BASED NANOCARRIERS FOR pH-RESPONSIVE DELIVERY OF ANTICANCER METAL COMPLEXES**

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Novel cancer-targeting nanotherapeutics are developed based on mesoporous silica nanoparticles (MSN) loaded with metal complexes, for potent activity against cancer. MSN was synthesized by surfactant-templated method. The nanomaterials are designed, through post-synthetic surface-functionalization, with capability to release Ruthenium- and Iridium-based drugs from MSN nanomaterials by lowering pH value. This effect would lead to preferential cancer targeting due to the more acidic tumor tissue in comparison to the healthy tissue. Novel Ru(II) and Ir(III) coordination compounds were also synthesized, containing the same ligands which are contained on the surface of MSN, and their anticancer activity was evaluated with and without their covalent attachment to MSN. The constructed series of novel nanomaterials and coordination compounds was characterized by scanning electron microscopy, thermogravimetric analysis, infrared spectroscopy, X-ray crystallography and elemental analysis. The characteristics of prepared metal complexes and novel nanomaterials demonstrate high potential for their effective application in targeted cancer treatment.

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## **STRUCTURAL, MORPHOLOGICAL AND ELECTRICAL PROPERTIES OF ALUMINA/YAG COMPOSITES AS SOLID ELECTROLYTE FOR IT-SOFC**

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Alumina/YAG composites (AYX<sub>t</sub>) with high relative density (99.2 %TD) were successfully obtained by mixing commercial alumina powder with different volume fractions of yttrium aluminium garnet (Y<sub>3</sub>Al<sub>5</sub>O<sub>12</sub>-YAG; 7, 14, 21 and 28). YAG was synthesized by nitrate glycine reaction in the form of precursor powder. Polycrystalline YAG powder was obtained by calcination at 950 °C for 2 h. Additionally, obtained compositions were characterized by XRD, SEM, EDX and electrochemical impedance spectroscopy. By XRPD analysis was found that the particle size of YAG powders lies in the nanometric range (being lower than 35 nm). By SEM microphotographs of composites were confirmed the formation of a conductive path consisting from mutually interconnected YAG particles. This was confirmed by the electrochemical impedance spectroscopy. The highest electrical conductivity of grain ( $\kappa_g$ ) and grain boundary ( $\kappa_{gb}$ ) at 700 °C amounted to  $2.22 \times 10^{-2} \Omega^{-1} \text{cm}^{-1}$  and  $9.44 \times 10^{-3} \Omega^{-1} \text{cm}^{-1}$ , respectively, was measured in the composite containing 21 vol.% of YAG.

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## PROPERTIES OF VARIOUS MULTIFERROICS PREPARED BY MIXING METHOD

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Multiferroic composites with formula  $\text{Ba}(\text{Ti}_{0.95}\text{Zr}_{0.05})\text{O}_3\text{--Ni}_{0.7}\text{Zn}_{0.3}\text{Fe}_2\text{O}_4/\text{CoFe}_2\text{O}_4/\text{Ni}_{0.7}\text{Cu}_{0.01}\text{Sm}_{0.05}\text{Zn}_{0.29}\text{Fe}_{1.95}\text{O}_4$  (BTZ(95-5)–NZF/CF/NCSZF) were prepared by mixing chemically obtained NZF, CF, NCSZF and BTZ(95-5) powders in the planetary mill for 24 h. All powders were prepared by the auto-combustion method starting from metal nitrates, titanium(IV) isopropoxide, zirconium(IV) oxynitrate and citric acid solution. Citric acid was added as a fuel and also as a complexing agent [1]. The optimization of sintering process was performed and the powders were pressed and sintered at 1250 °C for 4 h. X-ray measurements of obtained composites confirmed the presence of NZF, CF, NCSZF, BTZ(95-5) phases without the presence of any intermediate phases or impurities. Impedance analysis of all investigated samples has shown two semicircular arcs due to the presence of different relaxation processes that originated from the grain and grain boundary contributions. The results of polarization vs. electric field measurements have shown the influence of magnetic phases type and concentration on the ferroelectric properties of the composites. Due to high conductivity of ferrite phases and presence of interfacial polarization, the shapes of these curves differed from the conventional ferroelectric materials [2]. The values of remnant polarization were: 0.72, 0.34, 0.013  $\mu\text{C}/\text{cm}^2$  for the composites BTZ(95-5)-NZF, BTZ(95-5)-CF, BTZ(95-5)-NCSZF, respectively and for the saturation polarization were 1.2, 0.6 and 0.023  $\mu\text{C}/\text{cm}^2$ . In comparison with BTZ(95-5) this values are lower,  $P_r = 1.1$   $\mu\text{C}/\text{cm}^2$  and  $P_s = 4.5$ . However, due to the existence of non-saturated ferroelectric loops, the comparison of  $P_r$  and  $P_s$  was done at the appropriate field strength.

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## **TITANIA-BASED ELECTROSPUN NANOFIBERS AND THEIR PHOTOCATALYTIC PERFORMANCE**

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In this work we present detailed optimization of the titania-based electrospun nanofibers fabrication procedure. The starting solutions were prepared from stabilized titanium (IV) isopropoxide and different polymers, such as PCL (polycaprolactone) and PVP (polyvinylpyrrolidone). We report on the correlation between the processing parameters and functional properties of as synthesized fibers. Microstructural analyses performed on SEM and FE-SEM have revealed branchy morphology of nanofibers uniform in shape and size. Anatase phase in as prepared and calcined samples was disclosed by in-depth analysis of TEM images and SAED spectra. The obtained fibers were used in UV/Vis photocatalytic reactor for degradation of dye-contaminated water solutions. Promising results were observed showing improved behavior compared to referent samples. Furthermore, the influence of various dopants on the photocatalytic properties was investigated.

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## **Ag/TiO<sub>2</sub> NANOCOMPOSITE MATERIALS FOR APPLICATION IN VISIBLE-LIGHT PHOTOCATALYSIS**

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In this work we present novel and simple chemical method for preparation of Ag/TiO<sub>2</sub> nanocomposite powders and investigate their photocatalytic performance under visible irradiation (simulated AM1.5 spectrum). Presented method involves

usage of titanium(IV) isopropoxide, as titania precursor, and chitosan, as particles stabilizing agent and silver reduction agent. We present thorough characterization of the structural and optical properties, performed on the obtained powders by the means of FE-SEM, TEM, XRD, SAED, and UV-VIS-NIR spectroscopy. Microscopic analysis revealed the reduction of TiO<sub>2</sub> particles size upon the addition of silver into the system, and presence of sub-15 nm TiO<sub>2</sub> particles decorated with 3 nm-silver dots in the composite samples (0-10 wt.% of Ag). X-ray analysis disclosed single anatase phase in the samples calcined at 500 °C. The enhancement of visible light absorption was detected in all composite samples, compared to pure TiO<sub>2</sub> and referent commercial sample (Degussa P-25). Nanostructure of as synthesized silver nanodots was disclosed by in-depth analysis of recorded HRTEM images. Furthermore, we have observed superior photocatalytic behavior towards chosen organics-contaminated water solutions compared to the referent samples.

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## **FABRICATION OF CARBON-BASED ELECTRODES TRANSPARENT IN UV/VIS AND IR RANGE**

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Carbon nanotubes are undoubtedly among the most promising materials for development of transparent electrodes, due to their high electrical conductivity, good optical transparency and excellent chemical and mechanical stability. They can be processed in a form of a thin film via different techniques. Here, we have used layer-by-layer (LbL) assembly to form thin films of multi-walled carbon nanotubes (MWCNT). This technique has proven to be one of the best methods to prepare thin films from dispersion of carbon nanotubes. Thin films are formed by alternately depositing layers of oppositely charged MWCNT.

Two types of commercial MWCNT were used: MWCNT-COOH, with carboxylic groups and MWCNT-NH<sub>2</sub>, with amino groups. We deposited alternately layers of positively and negatively charged carbon nanotubes on different substrates (quartz, silicon). Dispersions of 0.1% of CNT were prepared using ultrasonic rod. Carboxylic nanotubes are stable in the water dispersion. However, amino nanotubes need additional surfactant to remain stable in the dispersion for a longer period. Therefore, sodium dodecyl sulfate was added as a stabilizer. Furthermore, we prepared also graphene oxide dispersion that we deposited via LbL technique after deposition of the layers of MWCNT. Addition of graphene oxide layer should increase the conductivity of MWCNT thin films. After the deposition of the

MWCNT and graphene oxide layers onto the substrates, samples were dried for 1 hour at 200 °C, and afterwards thermally treated in the vacuum at different temperatures, from 300 °C to 500 °C. Structural and morphological characterization of the films was analyzed with Raman spectroscopy and atomic force microscopy. Transmission of the samples was measured on UV/Vis spectrophotometer and FTIR. Transparency of the films in the infrared range was between 40 and 50%. Resistivity of the samples was measured, and it varied from 50 to 100 kΩ.

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### **INFLUENCE OF ZnO NANOPARTICLES ON SLOW RELEASE OF ESSENTIAL OIL FROM POLYMERIC MATRIX**

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Biopolymer emulsions were processed in the form of thin films for application in active food packaging. Active packaging is defined as material designed to release active components into food or absorb them from food in order to extend durability or to maintain/improve packaging conditions and extend shelf-life of food. We synthesized emulsion based on biodegradable polymers (pectin, gelatin, chitosan) with addition of active components -essential oils and ZnO nanoparticles (NPs). By introducing essential oils in the polymer matrix, with the addition of certain emulsifiers, it comes to encapsulation of oil droplets and the formation of a homogeneous emulsion. Thin films were fabricated by mold casting or spraying of the emulsions on a substrate. The slow release of an essential oil from the polymeric matrix was determined by UV-vis spectrophotometry. It was shown that polymers with addition of nanoparticles provided a prolonged action of active components. Surface morphology of the films was characterized by atomic force microscopy (AFM), and it was noticed that nanoparticles were mainly accumulated around oil droplets, which additionally contributed to a slow release of the active components.

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## MAGNETIC SPIN CHAINS IN COPPER(II) SUPRAMOLECULAR ARCHITECTURES

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Development of new technologies requires novel materials with desired chemical and physical properties which will have application in industry. Therefore, interest in molecule-based materials in recent years has increased because supramolecular assemblies exhibit many technologically important properties, especially in molecular magnetism based materials. In the study of molecular magnetism, magneto-structural correlations are of interest in which magnetic properties are analyzed in relation of local geometries, chemical linkages, bond length and angles, and close contact between magnetic species in the crystal packing. To elucidate influence of crystal packing on bulk magnetic properties it is necessary to design novel materials. [1]

With this in mind, we prepared a series of 1-D halide coordination polymers of copper(II) and amide derivatives of both pyrazine and pyrimidine. The targeted octahedral geometry was achieved for all structurally described complexes,  $[\text{CuCl}_2(2\text{-NH}_2\text{pz})_2]_n$ ,  $[\text{CuCl}_2(2\text{-pyz})_2]_n$ ,  $[\text{CuCl}_2(4\text{-pym})_2]_n$  and  $[\text{CuBr}_2(4\text{-pym})_2]_n$  and all obtained coordination compounds are distorted due to the Jahn–Teller effect. For all obtained coordination compounds temperature dependence of magnetization  $M(T)$  was measured using SQUID magnetometer in the temperature range 2–300 K. Linear dependence between magnetization and magnetic field allows usage of the linear magnetic susceptibility,  $\chi$ . Curie-Weiss model describes only paramagnetic behaviour in high temperature region, while at low temperatures all compounds exhibit a maximum in susceptibility. In accordance with crystal structure, we applied the more detailed approach of Bonner-Fischer and modelled entire  $M(T)$  curves for all obtained compounds using spin chain of antiferromagnetically interacting neighbouring  $\text{Cu}^{2+}$  ions along structural chains. Also, impact of the counter ion and Cu–X·Cu angles on superexchange interaction  $J$  is observed.

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**STRUCTURAL AND ELECTRO-MAGNETIC  
PROPERTIES OF Mg-DOPED POLYCRYSTALLINE  
 $\text{Bi}_{0.9}\text{Sm}_{0.1}\text{Fe}_{1-x}\text{Mg}_x\text{O}_3$  ( $x \leq 0.1$ ) FERRITES**

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Multiferroics are the materials which simultaneously exhibits two or more ferroic orderings like ferroelectricity, ferromagnetism and ferrotoroidicity at the same temperature [1]. Applications of these materials are in spin-electronics (spintronics) technology, such as the magnetic storage and sensors etc. It is proposed by many researchers that substituting rare earth elements at Bi and Fe sites in  $\text{BiFeO}_3$  may help to improve the ferroelectric and magnetic properties of BFO due to the volatilization of some reactants and phase decompositions at high temperature.

$\text{BiSm}_{0.1}\text{Fe}_{1-x}\text{Mg}_x\text{O}_3$  with  $x = 0, 0.025, 0.050, 0.075, 0.1$  are synthesized by the solid state method using high energy ball-mill. These powders are analyzed using the X-ray diffraction, field emission scanning electron microscopy (FESEM), and vibrating sample magnetometer (VSM). The dielectric constant and dielectric loss are measured by an impedance analyzer. A single perovskite  $R3c$  phase is found for BFO. The addition of Mg ion leads to the improvement of magnetization. Furthermore, the dielectric properties are improved as a result of reduction in  $\text{Fe}^{2+}$  and oxygen vacancies.

*Keywords:* bismuth ferrite, Mg-doping, magnetic properties, multiferroics

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**EFFECT OF CERIUM ( $\text{Ce}^{3+}$ ) DOPING ON STRUCTURAL,  
MAGNETIC AND DIELECTRIC PROPERTIES OF BARIUM  
HEXAFERRITE**

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Magnetic materials are comprehensively used as fundamental components for a large multiplicity of industrial and technological applications. Y-type hexagonal hexaferrites have grown much attention in recent years due to their multiferroic

properties. These ferrites are used in microwave devices, electronic communication, and various antenna components. The requirement of high-permeability and permittivity at relatively lower microwave frequencies considers Y-type hexaferrites as a potential material.

In the present work, the structural, magnetic and frequency dependent dielectric properties of the cerium doped barium hexaferrite are discussed. The sol-gel auto-combustion technique was employed for the preparation of these nano-hexaferrite catalysts. The crystallinity and phase purity of synthesized ferrite nanoparticles were confirmed by the X-ray diffraction technique. The magnetic and dielectric properties of the prepared samples were studied using SQUID based VSM technique and Impedance analyzer at room temperature. The magnetic study reveals that the saturation magnetization ( $M_s$ ) increases from 30.59 to 38.04 emu/g, whereas intrinsic coercivity ( $H_c$ ) increases from 19 to 118 Oe, with increasing doping level.

**Keywords:** hexaferrite, microwave, crystallinity, saturation magnetization, intrinsic coercivity

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### **MAGNETIC BEHAVIOUR OF Ag DOPED BiFeO<sub>3</sub>**

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Bismuth ferrite (BFO) is one of a few room temperature magneto-electric multiferroics. High ferroelectric and magnetic transition temperatures (1100 and 630 K, respectively) make it interesting for possible technological application. The problem with BFO bulk ceramic is low net magnetic moment of its ordered antiferromagnetic phase. To disturb the antiferromagnetic order and induce bigger magnetic moment, BFO is often doped with different elements, usually heavy rare earth elements or transition metal ions. In this study we have investigated magnetic behaviour of Ag doped BFO.

Compounds of BiFeO<sub>3</sub>, with metal ions substituted by different percentage of silver, were synthesized using hydrothermal method. Structural characterization of synthesized samples was performed using X-ray diffraction. Magnetization of polycrystalline samples measured in a wide temperature range, from 2 to 720 K, showed that the transition temperature for all the samples is nearly the same,  $T_N = 630$  K. The development of weak ferromagnetism with doping was observed as enhanced splitting between zero field cooled (ZFC) and field cooled (FC) curves, together with increased magnetization seen also in M(H) curves. The peculiar behaviour of ZFC and FC curves expressed at lower temperatures, where the FC curve crossed the ZFC curve attaining lower values of magnetization than the ZFC curve, could be attributed to the competition of exchange interactions within and between the sublattices.

*Acknowledgment:* The authors acknowledge the financial support of the Croatian Science Foundation under the project UIP-2014-09-8276.

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## **SYNTHESIS AND CHARACTERIZATION OF BiFeO<sub>3</sub> FINE POWDERS**

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Bismuth ferrite (BiFeO<sub>3</sub>) is one of the most studied multiferroic system with a large number of published articles. This is mainly because BiFeO<sub>3</sub> material possesses both ferromagnetic and ferroelectric properties observed at room temperature, which opens great possibility for industrial and technological applications. Well-crystallized single-crystal BiFeO<sub>3</sub> nanopowder has been successfully synthesized with the hydrothermal method. Structural analysis showed that non-annealed powder can be perfectly fitted to rhombohedral space group R3c and contains a very small amount of secondary phase, whereas the final product (annealed at 800 °C) represents single-phase perovskite powder with high crystallinity. HRTEM analysis confirmed existence of twin stacking faults, which are responsible for enhanced magnetic properties. EPR measurements suggested existence of electrons trapped by vacancies or defects. It has been proposed that existence of Fe<sup>3+</sup> –OV defect complex could be generated at elevated temperatures followed by formation of trivalent Fe ions, which intensely provide local 3d moments.

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## FERROELECTRIC, MAGNETIC AND RAMAN SPECTRA MEASUREMENTS OF $\text{Bi}_5\text{Ti}_3\text{FeO}_{15}$ AURIVILLIUS-BASED MULTIFERROIC MATERIALS

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One of the most important single-phase multiferroic materials with Aurivillius structure is  $\text{Bi}_5\text{Ti}_3\text{FeO}_{15}$  (BFT) which generally yields a magnetoelectric coupling above room temperature with a magnetoelectric coefficient of 10 mV/cmOe [1]. It has a special interest in this family of compounds because it is a combination of multiferroic  $\text{BiFeO}_3$  and ferroelectric  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$  and can be used as new magnetoelectric material for different devices. Years of intensive research have shown that the main lack of this material is high electrical conductivity and hence the low ferro-electromagnetic properties. This is a common problem in single-phase multiferroics, in general. Although they are expected to produce an applications breakthrough, they show poor properties at room temperature. Since BFT has the capability to host ions of different size, multiferroic properties could be improved by using dopants or ionic substitutions on different A and B-sites within the perovskite-like layers [2]. Insertion of magnetic ion such as  $\text{Co}^{3+}$  at B-sites could increase the remnant magnetization in BFT ceramics while  $\text{Y}^{3+}$  could enhance the dielectric and ferroelectric properties.

To this respect,  $\text{Co}^{2+}$  and  $\text{Y}^{3+}$  doped BFT were prepared by the solid state reaction method according to formulas:  $\text{Bi}_{1-x}\text{Y}_x\text{Ti}_3\text{FeO}_{15}$  ( $x = 0.1, 0.2, 0.3$ ) and  $\text{BiTi}_3\text{Fe}_{1-y}\text{Co}_y\text{O}_{15}$  ( $y = 0.1, 0.3, 0.5$ ). XRD data confirm the formation of single-phase Aurivillius compounds. SEM micrographs show an evident decrease in grain size of Co modified ceramics in comparison with pure BFT while there is no particular change of the grain size with Y doping. The ferroelectric and magnetic properties of all ceramic composites were also studied. Raman spectroscopy in dependence of temperature was used to give an insight to the possible ferroelectric character of BFT and also the way that dopants could influence the structural mechanism affecting the material's properties at the main magnetic and ferroelectric transitions.

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## ADJUSTING THE ELECTROLYTE PROPERTIES OF $\text{BaCe}_{0.9}\text{Y}_{0.1}\text{O}_{3-\delta}$ BY CO-DOPING

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Composition of  $\text{BaCe}_{0.9}\text{Y}_{0.1}\text{O}_{3-\delta}$  was changed by co-doping with 5 mole % of different cations ( $\text{In}^{3+}$ ,  $\text{Zr}^{4+}$  and  $\text{Nb}^{5+}$ ) to examine the influence of dopants on the electrolyte properties. The powder samples were synthesized by the citric-nitric autocombustion method.  $\text{BaCe}_{0.85}\text{Y}_{0.1}\text{In}_{0.05}\text{O}_{3-\delta}$  was successfully sintered at 1400 °C for 5 h in air, while a complete sintering of the other materials was carried out at 1550 °C. This makes the doping with In a preferable method since sintering temperatures below 1500 °C can limit BaO evaporation. The presence of In and Nb caused a significant drop in the total conductivity ( $\sigma$ ) of the ceramics at 700 °C in wet hydrogen, while the total conductivity of  $\text{BaCe}_{0.85}\text{Y}_{0.1}\text{Zr}_{0.05}\text{O}_{3-\delta}$  was slightly lower than of  $\text{BaCe}_{0.9}\text{Y}_{0.1}\text{O}_{3-\delta}$ . The stability of the ceramics exposed to a 100 %  $\text{CO}_2$  atmosphere at 700 °C for 5 h was investigated by X-ray analysis.  $\text{BaCe}_{0.85}\text{Y}_{0.1}\text{In}_{0.05}\text{O}_{3-\delta}$  showed considerable stability under the aggressive conditions containing traces of secondary phases, while the other samples were partially or significantly decomposed. By taking into account the factors that can influence the stability and conductivity, it was found that the dopant electronegativity had a decisive role both in inhibiting the carbonation and in decreasing the total conductivity of the ceramics.

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## **NANOINDENTATION STUDY OF Cu DOPED NaCo<sub>2</sub>O<sub>4</sub> CERAMICS**

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Thermoelectric materials, such as layered cobalt oxides, have been the subject of many theoretical and experimental investigations in past decade as potential candidates for application in energy conversion. In this work, polycrystalline samples of NaCo<sub>2-x</sub>Cu<sub>x</sub>O<sub>4</sub> (x = 0, 0.01, 0.03, 0.05) were synthesized from the powder precursors obtained by the citric acid complex method (CAC) and mechanochemically assisted solid state reaction method (MASSR). The obtained powders were uniaxially pressed into disc-shaped pellets and subsequently sintered at 880 °C in inert argon atmosphere. Indentation experiments were carried out to investigate mechanical properties. The hardness (H) and the Young's modulus of elasticity (Y) were determined using Agilent Nanoindenter G200. The surface approach velocity of the indenter (Berkovich pyramid) and Poisson ratio were set to 10 nm/s and 0.25, respectively. It was found that the highest Y (65.2 GPa) and H (1.41 GPa) were obtained for the CAC sample containing 1mol% of Cu. These results indicated a significant improvement of mechanical properties even in the case of the sample with the lowest dopant concentration.

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## STRUCTURAL, MICROSTRUCTURAL AND FERROELECTRIC PROPERTIES OF Ti-DOPED YMnO<sub>3</sub> CERAMICS SYNTHESIZED BY POLYMERIZATION COMPLEX METHOD

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Yttrium manganite, YMnO<sub>3</sub>, is a multiferroic material, which exhibits ferroelectric and antiferromagnetic behavior. These properties make it suitable for various applications [1]. Large microcracking and porosity in YMnO<sub>3</sub> ceramics strongly affect the material's ferroelectric response [2]. In this work, the effect of Ti doping on structure, microstructure and ferroelectric properties of YMnO<sub>3</sub> ceramics was investigated. The powders YMn<sub>1-x</sub>Ti<sub>x</sub>O<sub>3</sub> ( $x = 0; 0.10; 0.15; 0.20$ ) were prepared by polymerization complex (PC) method from citrate precursors, and calcined at 900 °C for 4 h. The ceramic samples YMnO<sub>3</sub> (YMO) and YMn<sub>0.9</sub>Ti<sub>0.1</sub>O<sub>3</sub> (YMTO10) were obtained after sintering at 1400 °C, YMn<sub>0.85</sub>Ti<sub>0.15</sub>O<sub>3</sub> (YMTO15) – at 1450 °C and YMn<sub>0.8</sub>Ti<sub>0.2</sub>O<sub>3</sub> (YMTO20) – at 1470 °C, for 2 h. Structural properties and phase composition of sintered samples were analyzed by X-ray diffraction (XRD) and their microstructure by scanning electron microscopy (SEM). Ferroelectric characterization was carried out by measuring of  $P(E)$  hysteresis loops and leakage current density ( $j_l$ ). XRD patterns of all ceramic samples revealed single-phased hexagonal ( $P6_3cm$ ) structure. It was observed that Ti-doped YMnO<sub>3</sub> ceramic samples have reduced microcracking, inter- and intragranular porosity. Leakage current densities of the samples YMTO10 and YMTO20 were lower compared to that of sample YMO. YMTO20 showed higher electrical conductivity, but all samples indicated weak ferroelectric response.

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**THE INFLUENCE OF SINTERING PROCESSING ON  
MICROSTRUCTURAL, OPTICAL AND ELECTRICAL  
PROPERTIES OF ZINC OXIDE CERAMICS  
DOPED WITH  $\text{Al}^{3+}$ ,  $\text{B}^{3+}$ ,  $\text{Mg}^{2+}$**

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Zinc oxide (ZnO) is a versatile functional material, widely employed in industry and technology as varistor ceramics, transparent conducting films, surface acoustic wave resonators etc. ZnO-based conductive ceramics, attractive for various applications, should have low electrical resistivity and good linearity. The n-type conductivity of wide band gap (3.37 eV) ZnO semiconductor could be enhanced by multiple doping with trivalent metals ( $\text{B}^{3+}$ ,  $\text{Al}^{3+}$ ,  $\text{Ga}^{3+}$ ,  $\text{In}^{3+}$ ), as shallow donors. The intrinsic defects, zinc vacancies and interstitial oxygen, exist in the grain boundaries of n-type ZnO ceramics as localized acceptor states. These states attract charge carriers, creating a depletion region around the grain boundaries and energy potential barrier, which hinder the motion of the electrons [1]. In this work, zinc oxide ceramics doped with  $\text{Al}^{3+}$ ,  $\text{B}^{3+}$  and  $\text{Mg}^{2+}$  was prepared using solid-state reaction technique from ZnO powder obtained in solvothermal synthesis and  $\text{Al}_2\text{O}_3$ , MgO and  $\text{B}_2\text{O}_3$  ( $\text{H}_3\text{BO}_3$ ) commercial powders.  $\text{Al}_2\text{O}_3$  was used as a donor dopant to increase the carrier concentration,  $\text{B}_2\text{O}_3$  was added to enhance densification and grain growth, and MgO – to decrease the thermal conductivity [2,3]. The pressed ZnO (0.25 %  $\text{Al}_2\text{O}_3$ , 0.5 %  $\text{B}_2\text{O}_3$ , 1 % MgO) pellets were sintered by conventional (CS) and spark plasma (SPS) method. The ceramic samples were analyzed by X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), UV-Vis spectroscopy and current-voltage (I–U) measurements. The correlation between the sintering processing, microstructure and electrical properties of multiple doped ZnO-based ceramics was investigated. The electrical performances of ZnO (0.25 %  $\text{Al}_2\text{O}_3$ , 0.5 %  $\text{B}_2\text{O}_3$ , 1 % MgO) ceramics were strongly dependent on composition and microstructure (density, grain size, segregation of secondary phase in grain boundaries). The electrical resistivity of SPS sample was an order of magnitude lower than electrical resistivity of CS sample and it showed almost linear I-U characteristics in temperature range of (25–150) °C.



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## **SBA-15 ASSISTED SnO<sub>2</sub> HUMIDITY SENSOR**

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Over the past decade, the interest for fabrication of mesoporous metal oxides has been increased, and that draw attention globally on fabrication and designing efficient humidity sensors based on these materials. Their unique properties like high surface area, large pore volume and interconnected pore channels provide easier adsorption and facile transportation of water molecules across their surfaces. Nanocasting as technique based on various silica hard templates is one of usually utilized and efficient methods for processing of such materials.

Silica SBA-15 as a template is currently obtaining exclusive attention in applications like photocatalysis, sensing, drug delivery and nanomaterials fabrication since it has high surface area, pore volume, excellent thermal stability and distinctive interconnectivity of its tunable pore channels. In this work, we used SBA-15 as a hard template for production of SnO<sub>2</sub> humidity sensor. SBA-15 assisted mesoporous SnO<sub>2</sub> has been synthesized using incipient wet impregnation process, consisting of two loading/calcination steps to fill up 15 % of the total pore volume of template with SnO<sub>2</sub>, followed by template etching with 2M NaOH.

A few micron thick SnO<sub>2</sub> film has been fabricated by applying the paste by the doctor blade applicator onto alumina substrate provided with interdigitated Pt/Ag electrodes. The sensor response of the film towards humidity was tested measuring the change of the complex impedance of the sample exposed to a humid climate chamber environment with the relative humidity, RH ranging from 40 % to 90 % at 25 °C and from 30 % to 90 % at 50 °C. This study demonstrated that nanocast SnO<sub>2</sub> possesses sufficient quality to be used as a material for fabrication of high performance humidity sensors.

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## SPARK PLASMA SINTERING OF CONDUCTIVE Sb-DOPED BaSnO<sub>3</sub>

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Barium stannate, BaSnO<sub>3</sub>, belongs to the group of perovskite-type alkaline earth stannates. It is an electrical insulator, but doping with proper cation can change its' electrical properties and transform it into an n-type semiconductor.

In this work, we present the Sb-doped barium stannate, BaSn<sub>1-x</sub>Sb<sub>x</sub>O<sub>3</sub>,  $x = 0.00, 0.04, 0.06, 0.08$  and  $0.10$  (labelled as BSSO<sub>x</sub>×100), using BaCO<sub>3</sub>, SnO<sub>2</sub> and Sb<sub>2</sub>O<sub>5</sub> as starting materials. Mechanically activated precursors were calcined at 900 °C for 4 h and subsequently sintered by Spark Plasma Sintering (SPS) Technique. For the characterization of obtained ceramic samples various techniques were used: X-ray Diffraction (XRD) analysis, High Resolution Transmission and Field Emission electron microscopy (HRTEM and FESEM) and UV-Vis spectroscopy. Electrical conductivity of BaSn<sub>1-x</sub>Sb<sub>x</sub>O<sub>3</sub> ceramic samples was determined by measuring the current-voltage ( $I-U$ ) characteristics in different mediums (air, silicon oil) at room temperature and temperatures up to 150 °C.

XRD analysis confirmed the formation of the cubic BaSnO<sub>3</sub> perovskite phase as a major, and tetragonal Ba<sub>2</sub>SnO<sub>4</sub> as a secondary phase. The content of Ba<sub>2</sub>SnO<sub>4</sub> phase decreased with introducing of Sb into the BaSnO<sub>3</sub> lattice. FESEM micrographs of fractured BaSn<sub>1-x</sub>Sb<sub>x</sub>O<sub>3</sub> ceramic samples showed well-densified microstructure and decrease of grain size with the increment of  $x$ . HRTEM analyses revealed the existence of low angle grain boundary (LAGB), which provides low energy conduction path of electrons. The results obtained from UV-Vis spectroscopy, indicated the decrease of band gap value of BaSn<sub>1-x</sub>Sb<sub>x</sub>O<sub>3</sub> samples with increasing Sb concentration. Electrical characterization confirmed that Sb-doped BaSnO<sub>3</sub> exhibits n-type conductivity. BaSn<sub>1-x</sub>Sb<sub>x</sub>O<sub>3</sub> samples with  $x = 0.04, 0.06, 0.08$  showed linear  $I-U$  characteristics at temperatures up to 150 °C. The highest electrical conductivity was 1.96 S/cm for the BaSn<sub>0.92</sub>Sb<sub>0.08</sub>O<sub>3</sub>. The increase of Sb concentration to  $x = 0.10$  led to the loss of  $I-U$  characteristics' linearity.

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## COMPARISON OF SENSING PROPERTIES OF SnO<sub>2</sub>/KIT-5 AND SnO<sub>2</sub> HUMIDITY SENSORS

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In this work, two different syntheses approaches – nanocasting and sol-gel technique were employed for the preparation of SnO<sub>2</sub> powders for humidity sensors. Stock solution of SnCl<sub>2</sub> in ethanol (0.5 M) was used as a Sn-precursor for both syntheses.

In the first procedure, this solution was infiltrated by wet impregnation method into the hydrothermally prepared KIT-5 used as silica template. Mesoporous SnO<sub>2</sub>/KIT-5 hybrid was obtained after two step loading/calcination process. Calcination was performed at 550 °C for 5 h. In the second procedure, silica template was excluded from synthetic path. Ethanol solution of SnCl<sub>2</sub> was slowly heated to form the gel which was later submitted to the same calcination conditions resulting in the preparation of SnO<sub>2</sub> nanopowder.

By dispersing the as prepared powders in the ethyl-cellulose/ $\alpha$ -terpineol solution and adding a few drops of acetic acid in the mixture, viscous pastes were prepared and further homogenized for 24 h with magnetic stirrer. Using doctor blade applicator a few micron thick films were deposited onto alumina substrates provided with interdigitated Pt/Ag electrodes.

Sensors' characteristics were compared by measuring the change of the complex impedance of the samples exposed to a humid climate chamber environment at different temperatures and RH values from 40 % to 90 % at 25 °C and from 30 % to 90 % at 50 °C. The value of impedance measured at 42 Hz and within the RH range of 40 % to 90 %, changes 53 times at 25 °C, and 96 times at 50 °C. In contrast, for the sensor prepared from chemically derived SnO<sub>2</sub>, the impedance changes in a moderate way – 8 times at 25 °C and 3 times at 50 °C. Fast response/recovery time of the SnO<sub>2</sub>/KIT-5 hybrid sensor exposed to humidity change from 40 % – 90 % at room temperature, confirmed superior potentials of this material for humidity sensing over the SnO<sub>2</sub>.

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## OPTIMIZATION OF MECHANICAL ACTIVATION OF FLY ASH

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More than 5.5 million tonnes of fly ash (FA), a by-product originating from coal combustion in thermal power plants (TPP), is produced in Serbia annually. Only small part of the FA is reused, mostly by cement industry, while the rest of it is disposed on landfills. Given its chemical composition and particle size distribution, FA has huge potential for reuse, especially in construction industry. Some of the most promising ways for FA utilization in building materials industry are synthesis of alkali-activated materials (AAM) and binders in which different quantities of Portland cement (PC) are substituted with FA (up to 80%). However, potential use of FA strongly depends on its reactivity. Among factors that affect FA reactivity, particle size distribution and amorphous phase content are the most important. A way to improve the reactivity of FA is mechanical activation, a process where mechanical energy is used to increase chemical reactivity of material. The main results of the mechanical activation process are particle size reduction, increase in specific surface area, generation of structural defects, increase in amorphous phase content, which all lead to better reactivity of material.

In this paper, FA from TPP “Kolubara”, Serbia, was mechanically activated in planetary ball mill using different ball-to-ash ratios, from 1:3 to 1:20. Characterization of raw and activated FA, such as particle size distribution, mineral and chemical composition, morphology and specific surface area, was carried out. The effects of mechanical activation of FA on the properties of resulting binders, both AAM and binder with PC, were also investigated.

It was found that mechanical activation, even with the lowest ball-to-ash ratio (1:3), caused drastic changes in particle size distribution and specific surface area of FA. Significant increase in compressive strength of mortars based on mechanically activated FA, relative to mortars based on raw FA, indicated that reactivity of FA was considerably improved by mechanical activation. Further increase in the ball-to-ash ratio led to less significant changes in the properties of the activated FA and therefore, less considerable increase in compressive strength of the synthesized mortars. It was concluded that, in terms of the balance between time and energy consumption, on the one hand, and improvement of the FA properties on the other, further increase of ball-to-ash ratios was not justified.

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## ROMAN METALLURGICAL VESSELS FROM MT. KOSMAJ

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Mt. Kosmaj, yield numerous evidences of Roman occupation during 2<sup>nd</sup>–4<sup>th</sup> century AD. It was an important cite for lead and silver production. Still many details about metallurgical activities that were accomplished during that time stay unresolved. Here we will present analyses of two remains of metallurgical activities excavated during archaeological researches in second half of 20<sup>th</sup> century. One is the litharge with remains of the vessel in which the cupellation was performed, found in one Roman grave G-253 at site of Guberevac [1], dated to the 2<sup>nd</sup> century AD. On the cross section of this find, there is visible contrast between inner red content with lead prills and outer brownish rather coarse layer also with metal prills. Another vessel is small grayish, bowl-shaped, with triangular rounded rim on the top and with white spots on the rim and outer side of the vessel, found in the Roman fortress of Stojnik.

The analyses are done with SEM-EDXRF for sample taken from litharge and with portable EDXRF for the metallurgical vessel. For litharge, results have shown that beside the presence of lead and minute amount of silver, some of the spectrums near the outer side, show signals for calcium and phosphorus. These elements indicate the technique of cupellation [2,3] that was done in porous cupels made of bone ore plant ash in order to separate silver from silver rich lead buttons from primary lead extraction process. Since there is no potassium found we can conclude that the bone ash was used for preparing the cupels. Another metallurgical vessel – small –greyish- round shaped shows signals of zinc, copper and lead besides the signals of iron, manganese and calcium attributed to clay minerals and calcite temper. This vessel was most probably used for diluting scraped brass with lead in order to obtain alloy suitable for casting. Similar vessels are reported at archaeological site *AUGUSTA RAURICA* in Switzerland [4].

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ISBN 978-86-80109-20-6