

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 of Excellence for Green Technologies, Institute for Multidisciplinary
Research, University of Belgrade
Faculty of Technology and Metallurgy, University of Belgrade

PROGRAMME and the BOOK of ABSTRACTS

6CSCS-2022

6th Conference of
the Serbian Society for Ceramic Materials
June 28-29. 2022. Belgrade Serbia

Edited by:
Branko Matović
Aleksandra Dapčević
Vladimir V. Srdić

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June 28-29, 2022

Belgrade, Serbia

6CSCS-2022

Edited by:
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Aleksandra Dapčević
Vladimir V. Srdić

SPECIAL THANKS TO



Република Србија

Министарство просвете,
науке и технолошког развоја



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- Institute for Multidisciplinary Research (IMSI), University of Belgrade
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WELCOME MESSAGE

On behalf of the organizers and organizing committee of the 6th Conference of the Serbian Society for Ceramic Materials (6CSCS-2022), I would like to extend my warmest welcome to all of you for attending the 6CSCS-2022. The conference is hosted and organized by the Serbian Society for Ceramic Materials, and co-organized by Institute for Multidisciplinary Research - 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 of excellence for green technologies, Institute for Multidisciplinary Research - University of Belgrade, and Faculty of Technology and Metallurgy - University of Belgrade.

The goal of the Conference is to provide 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 new direction for future development. 6CSCS-2022 aims to bring together leading academic scientists, researchers and research scholars to exchange and share their experiences and research results about all aspects of ceramic materials. It also provides the premier inter-multi-trans-disciplinary forum for researchers, practitioners and educators to present and discuss the most recent innovations, trends, and concerns, practical challenges encountered and the solutions adopted in the field of ceramic materials. We have received 75 abstracts with researchers from 17 countries.

The Conference will feature two plenary lectures, 16 invited talks and 57 oral and poster presentations as well as exhibitions of some new ceramic materials and devices. 6CSCS-2022 includes Ceramic powders, characterization and processing, High temperature phenomena, sintering, microstructure design and mechanical properties, Electro and magnetic ceramics, Ceramic composites, membranes and multimaterials, Traditional ceramics and Computing in materials science. Exhibitions from company sponsors will be held at the Conference as well.

We are grateful for the support from the Ministry of Education, Science and Technological Development of the Republic of Serbia. We would also like to express our sincere thanks to the symposia organizers, session chairs, presenters, exhibitors and all the Conference attendees for their efforts and enthusiastic support in this exciting time in Belgrade. I look forward to meeting you and interacting with you at Conference.

6CSCS-2022 President

Branko Matović

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6th Conference of the Serbian Society for Ceramic Materials
June 28-29, 2022, Belgrade, Serbia

PROGRAM of 6CSCS-2022

Day 1. Tuesday - June 28, 2022

08.00 – 09.00 h, Registration

09.00 – 09.15 h, Opening ceremony and welcome addresses

09.15 – 10.00 h, Cocktail

10.00 – 10.30 h, Plenary lecture, PL-1

Yuri Rostovtsev, *QUANTUM COHERENCE IN VARIOUS MATERIALS: TRANSPARENCY, HARMONIC GENERATION, QUANTUM CORRELATIONS, AND FREQUENCY DOWN CONVERSION*

Session 1: Ceramic Powders, Characterization and Processing

Chair: Zorica Branković, Claus Rebholz

10.30 – 10.50 h, Invited lecture, I-1

Claus Rebholz, *THERMAL AND CHEMICAL STABILITY OF BORON NITRIDE NANOSTRUCTURES*

10.50 – 11.10 h, Invited lecture, I-2

Sonja Jovanović, *THE STRUCTURAL AND MAGNETIC PROPERTIES OF COBALT FERRITE NANOPARTICLES: THE INFLUENCE OF HETEROATOMS*

11.10 – 11.30 h, Invited lecture, I-3

Matejka Podlogar, *SOLVOTHERMAL SYNTHESIS OF ZnO NANORODS FOR PHOTOCATALYTIC DEGRADATION OF ORGANIC POLLUTANTS*

11.30 – 12.00 h, Coffee break

Session 1: Ceramic powders, characterization and processing

Chair: Zorica Branković, Claus Rebholz

12.00 – 12.15 h, Oral presentation, O-1

Nikola Ilić, *NATURE OF PHOTOCATALYSIS IN BiFeO₃ SUSPENSIONS – HETEROGENEOUS, HOMOGENEOUS OR DYE-SENSITIZED?*

12.15 – 12.30 h, Oral presentation, O-2

Tamara Matić, *THE INFLUENCE OF HYDROTHERMAL SYNTHESIS TEMPERATURE OF MAGNESIUM DOPED HYDROXYAPATITE ON ITS APPLICATION AS DENTIN SUBSTITUTE*

12.30 – 12.45 h, Oral presentation, O-3

Tijana Stamenković, *THE INFLUENCE OF Yb³⁺ CONCENTRATION ON STRUCTURAL AND LUMINESCENT PROPERTIES OF Tm³⁺ DOPED SrGd₂O₄*

Session 2: Ceramic composites, membranes and multimaterials

Chair: Ravi Kumar, Vladimir Srdić

12.45 – 13.05 h, Invited lecture, I-4

Enikő Volceanov, *DEVELOPMENT OF ELECTROLESS Ni-P-NANOCOMPOSITE COATINGS ON LOW CARBON STEEL THIN STRIP*

13.05 – 13.20 h, Oral presentation, O-4

Irina Kandić, *CHARACTERIZATION OF ACTIVE CARBON MATERIALS OBTAINED FROM BIO WASTE FOR POTENTIAL USE IN WATER PURIFICATION*

13.20 – 14.45 h, Lunch break

14.45 – 15.30 h, Poster Session 1 (Posters P1 – P25)

Session 3: Electro and magnetic ceramics

Chair: Goran Branković, Slavko Bernik

15.30 – 15.50 h, Invited lecture, I-5

Slavko Bernik, *DEVELOPMENT AND CHARACTERISTICS OF A NOVEL ZnO-Cr₂O₃-BASED VARISTOR CERAMICS*

15.50 – 16.10 h, Invited lecture, I-6

Tomislav Ivek, *PROMOTION OF FERROMAGNETISM AND COLLAPSE OF VARIABLE-RANGE HOPPING TRANSPORT IN CERAMIC La_{0.5}Ca_{0.5}MnO₃ CONTROLLED BY GRAIN SIZE*

16.10 – 16.30 h, Invited lecture, I-7

Maria Čebela, *SYNTHESIS AND PROPERTIES OF MULTIFERROIC MATERIALS*

16.30 – 16.50 h, Invited lecture, I-8

Bojan Stojadinović, *SPIN-PHONON COUPLING IN NANOSTRUCTURES REVEALED BY RAMAN SPECTROSCOPY*

16.50 – 17.05 h, Oral presentation, O-5

Danica Piper, *BILAYER (La,Sr)MnO₃ AND (Ba,Sr)TiO₃ THIN FILMS PREPARED BY CHEMICAL SOLUTION DEPOSITION TECHNIQUES*

17.05 – 17.20 h, Oral presentation, O-6

Jelena Vukmirović, *EPITAXIAL GROWTH OF LaMnO₃ THIN FILMS BY POLYMER ASSISTED DEPOSITION TECHNIQUE ON THE DIFFERENT MONOCRYSTALLINE*

Day 2. Wednesday - June 29, 2022

09.00 – 09.30 h, Plenary lecture, PL-2

Ionescu Emanuel, *ADVANCED CERAMICS FOR ENERGY-RELATED APPLICATIONS: PRECURSOR-BASED SYNTHESIS & DESIGN CONCEPTS AND THEIR PERSPECTIVES TOWARDS SUSTAINABILITY*

Session 4: Computing in materials science

Chair: Yuri Rostovtsev, Dejan Zagorac

09.30 – 09.50 h, Invited lecture, I-9

K.C. Hari Kumar, *THERMODYNAMIC MODELLING OF Ta-N SYSTEM*

09.50 – 10.10 h, Invited lecture, I-10

Jelena Zagorac, *EFFECT OF ALUMINUM ADDITION ON THE STRUCTURE AND ELECTRONIC PROPERTIES OF BORON NITRIDE*

10.10 – 10.30 h, Invited lecture, I-11

Adrian Volceanov, *CHEMICAL BONDING IN CERAMICS AND GLASSES*

10.30 – 10.50 h, Invited lecture, I-12

Dejan Zagorac, *BARIUM SULFIDE UNDER PRESSURE: STRUCTURAL CHANGES, BAND GAP ENGINEERING AND MECHANICAL PROPERTIES*

10.50 – 11.05 h, Oral presentation, O-7

Dušica Jovanović, *ENERGY LANDSCAPE OF A RELAXED AMINO ACID, GLUTAMINE (L), ON TiO₂ SURFACES*

11.05 – 11.20 h, Oral presentation, O-8

Milan Pejić, *FIRST-PRINCIPLES INVESTIGATION AND STRUCTURE PREDICTION IN HOLMIUM(III) FLUORO-SELENIDE SYSTEM*

11.20 – 11.50 h, Coffee break

Session 5: High temperature phenomena, sintering, microstructure design and mechanical properties

Chair: Peter Tatarko, Branko Matović

11.50 – 12.10 h, Invited lecture, I-13

Peter Tatarko, *DEVELOPMENT OF HIGHLY TEXTURED DIBORIDE CERAMICS USING MAGNETIC AND ELECTRIC FIELDS*

12.10 – 12.30 h, Invited lecture, I-14

Ravi Kumar, *UNDERSTANDING DEFORMATION IN PRECURSOR DERIVED CERAMICS AT DIFFERENT LENGTH SCALES*

12.30 – 12.45 h, Oral presentation, O-9

Branko Matović, *SYNTHESIS AND CHARACTERIZATION OF HAFNIUM CARBIDE BASED CERAMICS*

12.45 – 13.00 h, Oral presentation, O-10

Jelena Vukašinić, *EFFECT OF THE SINTERING TECHNIQUE ON THE PROPERTIES OF Sb-DOPED BaSnO₃ CERAMICS*

Session 6: Traditional ceramics

Chair: Tatjana Volkov-Husović, Eniko Volceanov

13.00 – 13.20 h, Invited lecture, I-15

Jelena Maletaškić, *GLASS-CERAMICS OBTAINED FROM CAO-TiO₂-SiO₂ (SPHENE)*

13.20 – 13.40 h, Invited lecture, I-16

Tatjana Volkov Husović, *BLAST FURNACE REFRACTORIES: PAST, PRESENT AND FUTURE*

13.40 – 15.00 h, Lunch break

15.00 – 15.45 h, Poster Session 2 (Posters P26 – P47)

15.45 – 16.00 h, Marija Egerić, YOUNG CERAMISTS NETWORK

16.00 – 16.15 h, Closing ceremony

20.00 h, Conference dinner

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- P-1.** Tsvetan Dimitrov, *SYNTHESIS AND STUDY OF CHROMIUM-DOPED DIOPSIDE CERAMIC PIGMENTS*
- P-2.** Miluvka Stancheva, *STUDY OF CERAMIC PIGMENTS IN THE SYSTEM $\text{CaO} \cdot x(\text{REE}) \cdot (1-x)\text{MgO} \cdot 2\text{SiO}_2$*
- P-3.** Katarina Nikolić, *STRUCTURAL AND CHEMICAL PROPERTIES OF WASTE VITREOUS ENAMELS GENERATED DURING THE PRODUCTION PROCESS OF HEATING DEVICES*
- P-4.** Neda Nišić, *CHARACTERIZATION OF HIGH TEMPERATURE CERAMIC COMPOSITE SEALANTS (CCS) WITH ADDITION OF ALUMOSILICATE BASED WASTE MATERIAL FOR THE POTENTIAL USE IN IT-SOFC*
- P-5.** Marija Prekajski Đorđević, *SURFACE MODIFICATION OF CeO_2 NANOPOWDER*
- P-6.** Vladimir Dodevski, *SYNTHESIS OF OBTAINING SiO_2 FROM BIOMASS, CHARACTERIZATION OF STRUCTURAL AND CHEMICAL PROPERTIES AND THE POSSIBILITY OF POTENTIAL APPLICATION*
- P-7.** Katarina Vojisavljević, *HIERARCHICAL ZnO/SnO_2 HETEROSTRUCTURES VIA HYDROTHERMALLY ASSISTED ELECTROSPINNING TECHNIQUE: SYNTHESIS AND PHOTOCATALYTIC PERFORMANCES*
- P-8.** Andrijana Nedeljkovic, *XANTHATE ABSORPTION KINETICS AS A FUNCTION OF THE STARTING CONCENTRATION WITH THE USE OF THE WASTE SLAG AS ADSORBENT*
- P-9.** Božana Petrović, *BEHAVIOUR OF Mg and Si SUBSTITUTED HYDROXYAPATITES IN MODEL MEDIA*
- P-10.** Bojana Simović, *IMPROVED PHOTOCATALYTIC DEGRADATION OF RO16 DYE USING HYDROTHERMALLY SYNTHESIZED $\text{CeO}_2 @ \text{ZnO}$ NANOCOMPOSITE*
- P-11.** Jelena Jovanović, *VISIBLE-LIGHT PHOTOCATALYTIC DEGRADATION OF MORDANT BLUE 9 BY BiVO_4 NANOPOWDER*
- P-12.** Milena Rosić, *INVESTIGATING SORPTIVE ASPECTS OF CoMoO_4 NANOPOWDERS SYNTHESIZED BY SPR METHOD*
- P-13.** Ivan Stijepović, *ION MIGRATION IN SPINEL STRUCTURE IN NICKEL AND ZINC FERRITE NANOPOWDERS SYNTHESISED BY CO-PRECIPIITATION AND HYDROTHERMAL METHODS*

P-14. Aleksandar Malešević, *STABILITY AND FUNCTIONALITY OF BaCe_{1-x}In_xO_{3-δ} AS A HIGH TEMPERATURE PROTON CONDUCTING ELECTROLYTE FOR SOLID OXIDE FUEL CELLS*

P-15. Marija Egerić, *ENHANCED PHOTOCATALYTIC REMOVAL OF CONGO RED BY MOF-ACTIVATED CARBON COMPOSITE*

P-16. Marija Egerić, *COMPETITIVE REMOVAL OF DIVALENT HEAVY METAL IONS FROM SYNTHETIC AND REAL WASTEWATER BY ARAGONITE SEASHELL WASTE*

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P-18. Tijana Stamenković, *SURFACE CHARACTERIZATION AND PHOTOCATALYTIC ACTIVITY OF NEWLY SYNTHESIZED DY DOPED SrGd₂O₄ PHOSPHORUS*

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P-33. Nenad Nikolić, *THE COMPARISON OF ELECTROCHEMICAL PROPERTIES OF ZnMn₂O₄ AND ZnCr_{0.15}Mn_{1.85}O₄ IN AN AQUEOUS SOLUTION OF ZnCl₂*

P-34. Danijela Luković Golić, *THE IMPROVEMENT OF FERROELECTRIC PROPERTIES OF BiFeO₃ CERAMICS BY DOPING WITH La³⁺ AND Eu³⁺*

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P-40. Milan Pejić, *ENERGY LANDSCAPE EXPLORATION OF NOVEL TERNARY RARE-EARTH COMPOUND LAIO*

Poster session 5: High temperature phenomena, sintering, microstructure design and mechanical properties

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P-44. Robert Vigi, *THERMAL PROPERTIES OF Ag DOPPED GLASS-CERAMIC MATERIAL FROM As-Te-Se SYSTEM*

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P-45. Jelena Rakić, *EFFECT OF TWO ACTIVATION METHODS ON MECHANICAL PROPERTIES OF HIGH VOLUME FLY ASH BINDERS*

P-46. Zvezdana Baščarević, *SYNTHESIS OF GEOPOLYMERS BASED ON SPENT CATALYST FROM PETROL REFINERIES*

P-47. Aleksa Luković, *DETERMINING THE ABSOLUTE AGE AND TYPE OF MAGMA OF TRIASSIC ANDESITES OF ČADINJE USING U/PB DATING AND BACKSCATTER METHODS ON ZIRCON SAMPLES*

PL-1

**QUANTUM COHERENCE IN VARIOUS MATERIALS:
TRANSPARENCY, HARMONIC GENERATION, QUANTUM
CORRELATIONS, AND FREQUENCY DOWN CONVERSION**

Yuri Rostovtsev

*Department of Physics and the Center for Nonlinear Sciences,
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Basic properties of materials can be enhanced by the quantum coherent effects such as electromagnetically induced transparency, coherent population trapping, and induced large Kerr nonlinearities. The quantum coherence effects can be used to develop a bright compact source for entanglement photons that can have broad applications to quantum information and high-precision spectroscopy. In particular, the localized plasmon interaction in quantum confined structures strongly modify the optical and electronic properties with potential for manipulating light on the nanoscale. The strong excitonic absorption in 2D semiconductors enables enhanced nonlinear optical interactions due to strong exciton-plasmon coupling to demonstrate quantum coherent and cooperative effects near the surface of plasmonic metamaterials as manifestation of the super-radiant and sub-radiant Dicke states. We have demonstrated the quantum coherent effects that are able to have an all-optical control on ultrafast time scales, over the photonic topological transition, for applications to quantum sensing, quantum information processing, and quantum simulations using metamaterials.

PL-2

**ADVANCED CERAMICS FOR ENERGY-RELATED
APPLICATIONS: PRECURSOR-BASED SYNTHESIS & DESIGN
CONCEPTS AND THEIR PERSPECTIVES TOWARDS
SUSTAINABILITY**

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In the present talk, various precursor-based synthesis concepts for ceramics and ceramic nanocomposites to be used in advanced structural and functional applications will be presented and critically discussed. Within this context, emphasis will be put on single-source-precursor-based approaches for ceramic materials with tailored and predictable phase compositions and property profiles. Also, selected examples of ceramic materials development for specific energy conversion and storage applications will be highlighted. Furthermore, the presented synthesis and design concepts will be discussed with respect of their implications in the sustainability of ceramics. Thus, the talk will elaborate on the high potential and unique perspectives of precursor-based synthetic approaches for realizing innovative solutions towards a circular economy in ceramics.

I-1

THERMAL AND CHEMICAL STABILITY OF BORON NITRIDE NANOSTRUCTURES

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In recent years, there has been a great interest in the synthesis and application of boron nitride (BN) nanomaterials due to their unique physical, chemical and mechanical properties. Much attention has been drawn towards nanoscale h-BN, among the most promising inorganic nanomaterials. In this study, the texture/porosity, structure, surface chemistry, morphology and elemental composition of h-BN nanoplatelets and nanotubes were evaluated and compared to carbon-based materials with similar structures. The experimental results showed superior high temperature stability for the h-BN nanomaterials and revealed which of the evaluated materials demonstrated the best high-temperature performance/resistance, therefore allowing the correlation of oxidation behaviour with specific structural features (e.g. crystallinity, specific surface area, particle shape).

I-2

THE STRUCTURAL AND MAGNETIC PROPERTIES OF COBALT FERRITE NANOPARTICLES: THE INFLUENCE OF HETEROATOMS

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In the last two decades the magnetic nanoparticles have been widely applied in data storage, catalysis, energy, environment, and in particular, biomedicine. For each application, the magnetic nanoparticles with pre-defined properties are required. However, the synthesis of such nanoparticles is often challenging due to various parameters that influence their physicochemical properties.

In this talk, a case of cobalt ferrite nanoparticles (CFO NPs) will be presented in which solvothermal method was used for designing non-agglomerated particles with uniform morpho-structural properties. It will be described how the uniformity of size and shape distribution can be attained for the purpose of enabling more detailed insight into the role of heteroatoms on the magnetic properties of CFO NPs.

The talk will address the positive role of oleic acid in the synthesis of non-agglomerated, sphere-like particles, with uniform size distribution – a prerequisite for the investigation of the influence of heteroatoms on physicochemical properties of CFO NPs. This will be done from the point of view of optimal concentration of oleic acid and the nature of its bonding to the surface of nanoparticles. Finally, it will be discussed how substitution of Co^{2+} and Fe^{3+} with Zn^{2+} and Ga^{3+} , respectively, can be used for tuning the magnetic properties of spinel ferrites for specific applications.

I-3

SOLVOTHERMAL SYNTHESIS OF ZnO NANORODS FOR PHOTOCATALYTIC DEGRADATION OF ORGANIC POLLUTANTS

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Nano zinc oxide (ZnO) gained a lot of attention for photocatalytic applications and is frequently used to degrade many organic pollutants in water, from dyes to microplastics. Photocatalysis, is a chemical oxidation processes, where commonly nanostructured semiconductor (photocatalyst) is irradiated with an appropriate light energy to create electron-hole pairs, that react with the surrounding water and produce superoxide and hydroxyl radical that can oxidize given chemical species/pollutant. As photocatalysis is an exclusively surface driven process, its activity depends on the particle size, specific surface area and morphology of the used photocatalyst. Nanostructured materials with high surface to volume ratio have high photocatalytic degradation efficiency.

Nano ZnO can be prepared with many different techniques. In our study, first nanodots of ZnO were prepared. After the distillation of Zn-acetate ethanol solution, ZnO nanoparticles were precipitated by the addition of LiOH. Further solvothermal treatment, in autoclave at 150 and 200 °C for 24 or 120 h, transformed nanodots to nanorods. Synthesized nanopowders were characterized using X-ray diffraction analysis (XRD), Raman spectroscopy, scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The photocatalytic activity of prepared ZnO nanostructures was investigated by caffeine and molybdenum blue degradation. These common pollutants were dissolved in miliQ water with concentration of 10 mg/L. The photocatalytic degradation was carried out in cylindrical reactor with quartz cover, where 5 mg of photocatalyst was added to 5 mL of solution. Before irradiation, samples were kept in the dark for 60 min to reach the adsorption desorption equilibrium. Suspensions of ZnO in pollutant solution were irradiated under stirring using a UV-vis simulated sun spectrum (Ultra Vitalux, 300 W, Osram). At pre-defined time intervals, the caffeine/MB concentration was analyzed by spectrophotometer (Lambda 950 UV/Vis/NIR, PerkinElmer). We correlate the obtained degradation rate with the crystallinity, crystal size, aspect ratio, specific surface area and structural and surface defects. Nanorods solvothermally synthesized at 200 °C for 24 h showed the highest photocatalytic activity, and consequently we tested them also for photocatalytic degradation of synthetic microfibers (PET, PA). SEM and Raman analysis, after the exposure by simulated sun light irradiation, showed changes on surface of plastic fibers.

I-4

DEVELOPMENT OF ELECTROLESS Ni-P- NANOCOMPOSITE COATINGS ON LOW CARBON STEEL THIN STREEP

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Nickel-phosphorus (Ni-P) coatings can be widely used in many industrial applications due to their outstanding mechanical and chemical properties, such as high hardness and good corrosion and wear resistance [1,2]. Ni-P coatings can be manufactured using a variety of techniques, including electroplating and electroless chemical deposition. Metals can be protected from wear (abrasion) by covering them with metal matrix composites containing ceramic particles such as: Al₂O₃, TiO₂, SiO₂, ZrO₂, SiC, Si₃N₄, B₄C, WC, etc. On the other hand, these hard materials are too fragile and offer little or no adhesion for use as a coating. Therefore, a metal matrix is used to hold the oxide particles together and to facilitate good adhesion to the coated metal surface. However, the chemical method is a method usually applied on parts; the continuous steel strip coating has a high drawback, namely the low speed layer deposition. Our investigations were focused on enhancing the deposition speed and homogeneity. Two bath compositions were developed for the electroless deposition, namely Bath (A): composed of nickel sulphate and sodium hypophosphite aqueous solutions and various admixtures (sodium acetate, ammonium sulphate, sodium citrate, sodium dodecyl sulphide and lead acetate) and Bath (B): Bath (A) to which nanosized oxide particles was added in various amount in the range of 2–20 g/L. The deposition rates, co-deposition of particles, roughness were influenced by the nanopowders concentration, temperature, agitation rate, and pH and deposition duration in the bath. After deposition the coating is amorphous. The change in hardness with heat treatment exhibits a similar trend for these coatings, which suggests that the hardening mechanism upon annealing is the same for both electroless Ni-P and Ni-P-nanocomposite coatings. Increase in hardness up to 400 °C is due to precipitation hardening because of the formation of the intermetallic Ni₃P phase. The decrease in lattice defects and coarsening of the Ni₃P particles cause a reduction in hardness when these coatings were annealed beyond 400 °C. The adhesion and uniformity of the composite layers, analyzed metallographically and by SEM are appropriate, so the interface of the composite layer with the support steel is perfectly continuous, without discontinuities and the layer is uniform.

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I-5

DEVELOPMENT AND CHARACTERISTICS OF A NOVEL ZnO-Cr₂O₃-BASED VARISTOR CERAMICS

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Exceptional current-voltage (I - U) nonlinearity with a high energy-absorption capability makes ZnO-Bi₂O₃-based varistor ceramics a cornerstone of commercial varistor materials for overvoltage protection. Recently we discovered a novel, sustainable, ZnO-based varistor ceramic, which is based on Cr₂O₃ as the varistor former and oxides of Ca, Co and Sb as a performance enhancer. Compared to previously known ZnO-based varistor ceramics, this novel ceramic does not contain the highly volatile Bi₂O₃, expensive rare-earth elements (Pr₆O₁₁) or toxic V₂O₅, and the microstructure is practically single-phase. The discovery of the ZnO-Cr₂O₃-based varistor ceramic represents a major breakthrough in the field of varistors and could drastically affect the world market for overvoltage protection.

The ZnO-Cr₂O₃-based varistor ceramic has a high coefficient of nonlinearity (α) up to 219, a low leakage current (I_L) below 0.2 $\mu\text{A}/\text{cm}^2$, and a breakdown voltage (E_b) from 400 to 925 V/mm. The design of this novel varistor ceramic, by tailoring states at the grain boundaries of ZnO, leading to the formation of electrostatic Schottky barriers with the addition of Cr₂O₃ and superior current-voltage characteristics of ceramics, will be presented and discussed.

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I-6

**PROMOTION OF FERROMAGNETISM AND COLLAPSE OF
VARIABLE-RANGE HOPPING TRANSPORT IN CERAMIC
 $\text{La}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ CONTROLLED BY GRAIN SIZE**

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Manganites have attracted attention of applied and fundamental research alike since the discovery of colossal magnetoresistance – the dramatic change in electric conductivity under applied magnetic field. This effect is closely related to the competition between the ferromagnetic metallic phase and the antiferromagnetic charge-ordered insulator with localized electrons and a long range order. While the metallic phase is considered to be well understood, the exact origin of the insulating behavior in manganites is still the subject of active study.

Here we report on a low-temperature dc resistivity and magnetization study of manganite $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ ceramic samples at the boundary between charge-ordered/antiferromagnetic insulating and ferromagnetic metallic phases, $x = 0.5$. By varying the grain size, we observe disorder-induced changes in magnetic response and the predominant charge transport mechanism. Significant increase of disorder associated with the reduction in grain size pushes the system towards metal-like behavior, quite the opposite from what is expected within a naive Anderson localization scenario. The obtained results are discussed in light of strong electron-lattice coupling as a necessary ingredient in understanding electron localization effects in manganites.

I-7

SYNTHESIS AND PROPERTIES OF MULTIFERROIC MATERIALS

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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. BiFeO₃ and Bi_{1-x}Ho_xFeO₃ 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 Ho³⁺ ions in the BiFeO₃ crystal lattice, where they substitute Bi³⁺ 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 BiFeO₃ compounds produced in the experiment. Magnetic behavior 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.

I-8

SPIN-PHONON COUPLING IN NANOSTRUCTURES REVEALED BY RAMAN SPECTROSCOPY

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The knowledge of the subtle interplay between the spin and lattice degrees of freedom (spin-phonon coupling) presents an important aspect in manipulating the magnetic, ferroelectric and magneto-electric properties of composite nanostructures.

Spin-phonon interaction in magnetic nanostructures most often manifests as non-typical temperature dependence of optical phonons frequencies, since phonon energies can be influenced by the exchange coupling between magnetic ions at and below the temperatures of magnetic phase transitions. Due to the complexity of magnetic interactions in nanomaterials, the coupling between the lattice vibration and the magnetic order can be different for different phonon modes and the coupling strength may vary even in the case of the same spin-spin interaction. Raman spectroscopy is a very powerful technique to elucidate the spin dynamics and the effects of the interaction of optical phonons with different magnetic ordering. More or less phonon frequency deviation from anharmonic behaviour manifests in the Raman spectra as positive/negative frequency shift below magnetic ordering temperature and is dependent on the relative strength of antiferromagnetic (AFM) or ferromagnetic (FM) exchange interaction. From this shift it is possible to derive estimates for the spin-phonon coupling strength.

The spin-phonon coupling mechanism will be demonstrated on the example of two different magnetic nanomaterials, antiferromagnetic bismuth ferrite, BiFeO_3 , and ferrimagnetic iron garnet, $\text{Dy}_3\text{Fe}_5\text{O}_{12}$. The spin-phonon interaction in these materials was explained within the mean field approach which enabled to extract the spin-spin correlation function and in addition allowed a quantitative assessment of the spin-phonon coupling strength for different phonon modes.

I-9

THERMODYNAMIC MODELLING OF Ta-N SYSTEM

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Tantalum nitrides have great promise as potential candidates for several technological applications that require high hardness, high mechanical strength, good thermal stability, good chemical stability, high melting point, low electrical resistivity, good diffusion barrier properties, superconductivity, and the right band gap [1]. We report the thermodynamic of Ta-N using the CALPHAD approach combined with first-principle calculations. The present study includes the thermodynamic modelling of the nitrides δ -TaN (cF8), Ta₂N (hP9), ϵ -TaN (hP6), and α -Ta₃N₅ (oC32).

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I-10

EFFECT OF ALUMINUM ADDITION ON THE STRUCTURE AND ELECTRONIC PROPERTIES OF BORON NITRIDE

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The influence of the structure type on the boron nitride (BN) properties such as excellent thermal and chemical stability and super hardness is well known. A detailed study of the structural and electronic properties of the $B_{1-x}Al_xN$ solid solutions for $x = 0, 0.125, 0.25, 0.375, 0.5$, has been conducted on *ab initio* level. Prediction of four structure candidates has been performed in each of the possible compositions using hybrid B3LYP functional, resulting in interesting AlN-BN compounds with unique properties. In the case of the pure BN, our results are in agreement with previous experimental and theoretical data. For the not-yet synthesized $B_{0.825}Al_{0.125}N$ compound, all modifications become slightly distorted except rock-salt, which has been converted to the GeP phase. With further increase of the Al in the system, we have investigated $Al_{0.75}B_{0.25}N$ composition and all modifications become highly distorted, with h-BN becoming an unknown type of structure. With 37.5% of Al in the system, we observe fewer distortions in the structure, including AlN and BN layer separation in the structures, which is completely obtained with 50% of aluminum in boron nitride. Also, we note that the wurtzite modification is the energetically most favorable minimum regardless of aluminum concentration. Moreover, boron nitride is much less investigated for its semiconducting properties and the possible effect of aluminum addition to the BN. We have found various band gap sizes and the possibility to tune direct/indirect band gap using various predicted modifications. In principle, the highest band gap values are encountered in the wurtzite-related structures regardless of composition, and the band gap is generally reduced with the increase of aluminum in the structure. Present results suggest that there is a great diversity of the electronic properties caused by adding aluminum to boron nitride and that by using these additional four modifications per investigated $B_{1-x}Al_xN$ ($x = 0; 0.125; 0.25; 0.375; 0.5$) composition, one could tune the band gap of boron nitride electroceramics for industrial, scientific, and/or technological applications.

I-11

CHEMICAL BONDING IN CERAMICS AND GLASSES

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Oxide materials are interesting from both a theoretical and technological point of view, especially since they can have important electrical, electronic, magnetic, optical, and catalytic properties. The ionic-covalent character of the metal-to-oxygen bonding in metal oxides influences the physical and chemical properties of the technologically important materials. While the nature of the cohesive forces in fully covalent or fully ionic compounds is well established, there was until recently a lack of conceptual basis to describe it in mixed ionic-covalent materials. The understanding of how the competition between ionic and covalent processes fixes the anion-cation electronic-sharing, the characteristics of the energy bands and the cohesive energy is incomplete, both from the experimental and theoretical points of view.

Present paper deals with a novel approach on theoretical ionicity / basicity based on electronic energy levels or band structure of solids. Our approach is based mostly on experimental data, available in literature, but with a better understanding of the physical-chemical meaning of the concept. The obtained results are similar to those reported in literature but computed with more sophisticated methods. Making appropriate assumptions our approach can be applied to non-ordered structures, as well. Another major adjustment considers the possibility of decomposing ionicity of complex chemical bondings into a sum of binary bondings as suggested by Zhang and co-workers.

Applications of ionicity for different ceramic materials and glasses are presented. Thus, there are given results for hardness, polymorphs, etc. The variation of ionicity (basicity) with temperature is also presented, this finding being able to open a new view on thermal behaviour or thermal history of ceramics/glasses considered through chemical character of bondings.

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I-12

BARIUM SULFIDE UNDER PRESSURE: STRUCTURAL CHANGES, BAND GAP ENGINEERING AND MECHANICAL PROPERTIES

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Barium sulfide (BaS) is an important precursor to other Ba compounds with applications from ceramics and flame retardants to luminous paints and additives, and recent research shows numerous potential technological applications. Under normal conditions, BaS crystallizes in the NaCl type of structure, and with the increase in pressure BaS undergoes a structural phase transition to a CsCl type modification. Density Functional Theory (DFT) study has been performed in order to investigate behaviour of BaS at high pressures, and relationship between computed properties [1]. Novel predicted and previously synthesized BaS modifications have been calculated using Local Density Approximations (LDA) and Generalized Gradient Approximation (GGA) functionals. A detailed investigation of structural changes and its corresponding volume effect up to 100 GPa, with gradual pressure increase, has been performed from the first principles. Band gap engineering of the experimentally observed BaS phases at high pressures has been simulated and structure-property relationship is investigated. For each of the predicted and experimentally observed BaS structures, elastic constants and mechanical properties under compression have been investigated (e.g. ductility/brittleness, hardness, anisotropy) [2,3]. This study offers a new perspective of barium sulphide as a high pressure material with application in ceramics, optical and electrical technologies.

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I-13

DEVELOPMENT OF HIGHLY TEXTURED DIBORIDE CERAMICS USING MAGNETIC AND ELECTRIC FIELDS

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Highly textured TiB₂ ceramics were prepared by slip casting an aqueous suspension in a magnetic field of 9 T, followed by sintering using Field Assisted Sintering Technology (FAST). Particle size refinement by ball milling improved both the degree of texturing and densification of the material ($RD > 98$ %TD). The sintered material exhibited a Lotgering orientation factor of 0.90, with the *c*-axis of TiB₂ oriented parallel to the magnetic field and FAST pressing direction. The effect of pressing direction was negligible. The textured TiB₂ material exhibited a significant anisotropy in mechanical properties; the values of hardness and elastic modulus measured along directions transverse to the *c*-axis of TiB₂ were 37 % and 13 % higher than the ones measured along the *c*-axis direction. Moreover, the specific wear rate of a surface of textured TiB₂ parallel to the field was one order of magnitude lower than a surface perpendicular to the field.

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I-14

UNDERSTANDING DEFORMATION IN PRECURSOR DERIVED CERAMICS AT DIFFERENT LENGTH SCALES

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Polymer precursor route for the synthesis of advanced ceramics has attracted considerable interest due to their exceptional high temperature stability, resistance to crystallization, phase separation and creep. More recently these ceramics were considered as suitable materials for applications such as in micro- and nano-electro mechanical systems (MEMS/NEMS). In view of this it is of importance to understand the deformation behavior of these ceramics at micro- to nanoscale loads. In this study the deformation behaviour of the PDCs were captured using depth sensing nanoindentation and compared with micro-indentation techniques. A plastic work ratio of less than 0.5 was observed in all PDCs and hence it is suggested that the deformation occurs mainly by sink-in. The load-displacement curves exhibited very high elastic recovery with an elastic work ratio of 0.71. The elastic modulus of these PDCs varied between 105 and 310 GPa and indentation hardness was varied between 5 GPa and 20 GPa. The variation in hardness and elastic modulus is assigned to the difference in the chemical bonding of each of these polymer derived ceramics. In recent times, we have also attempted to understand the deformation behavior using a home-built universal testing machine with *in situ* characterization capabilities and some of the preliminary results shall be discussed as well.

I-15

**GLASS-CERAMICS OBTAINED FROM CAO-TIO₂-SIO₂
(SPHENE)**

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Sphene based glass-ceramics (CaTiSiO₅), an excellent candidate for a host lattice of ceramic materials and for nuclear waste immobilization, has been prepared from a powder mixture of CaCO₃, TiO₂ and SiO₂ using vibro-milling for homogenization. Starting powders were melted at 1400 °C for 2 h, cooled to room temperature, grounded again, and then crystallized by thermal treatment yielding a sphene glass-ceramic. The evolution of the phase composition during thermal treatment was investigated by X-ray powder diffraction (XRPD), FT-IR, Raman and thermal analyses (TG-DTA). Pure synthetic single phase sphene was formed at 800 °C for 4 h, even if is very hard to obtain monophasic powder at such low temperature. Powder morphology was analyzed by scanning electron microscopy (SEM).

I-16

BLAST FURNACE REFRACTORIES: PAST, PRESENT AND FUTURE

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Most of the refractories used today are related to iron and steel industry. Grate part of the refractory lining related to blast furnace are combination of different refractory materials selected for different parts of furnace, as well as different process conditions and temperature range. Selection of appropriate refractory combination depends on knowledge and demands for iron making system in combination with the physical, mechanical and chemical properties of the proposed refractories. An improper understanding of the above factors often leads to a refractory failure which, subsequently, becomes a complex problem to solve. Refractory linings whether it is of a blast furnace or any other furnace, usually fail due to any number or combination of such factors. For the convenience of understanding, here we will discuss the types of refractory lining required in a blast furnace area as well as the trend in the refractory lining pattern that has been used during the last decades.

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O-1

**NATURE OF PHOTOCATALYSIS IN BiFeO₃ SUSPENSIONS –
HETEROGENEOUS, HOMOGENEOUS OR DYE-SENSITIZED?**

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Bismuth ferrite (BiFeO₃) powders were synthesized by auto-combustion method. To decrease the quantity of active phase and improve the specific surface area, composites of BiFeO₃ and natural porous materials (diatomaceous earth and cuttlebone) were prepared by chemical method from solution and calcined at low temperature. Such obtained powders were used as adsorbents and photocatalysts in methylene blue water solutions. Nature of photocatalysis under visible and UV-Vis light was examined under different pH conditions and presence of hydrogen peroxide, dissolved iron(III), oxalates and some other ions. Methylene blue is capable to absorb sunlight and insert electrons into semiconductor, so possibility of this way achieved dye-sensitization was studied [1]. Composites expressed better properties than individual components confirming the synergetic effect [2]. Acidic conditions were more suitable for decolorization, so possible Fenton reaction based homogeneous catalysis was also considered.

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O-2

THE INFLUENCE OF HYDROTHERMAL SYNTHESIS TEMPERATURE OF MAGNESIUM DOPED HYDROXYAPATITE ON ITS APPLICATION AS DENTIN SUBSTITUTE

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The needle-like morphology of hydrothermally obtained nanosized hydroxyapatite powders mimics biological apatite, the main mineral component of human bones and teeth. Since the apatite in nature contains many impurities in its structure, such as Mg²⁺, Sr²⁺, Cu²⁺, F⁻, etc. the ion-doping approach has been proposed as a possible path for mimicking the mineral component of hard tissue for bone and teeth tissue repair and regeneration. Previously, the undoped hydroxyapatite-based compacts were shown to be adequate dentin substitutes for application in restorative dentistry.

The aim of this study was to analyze the influence of synthesis temperature during hydrothermal synthesis of nanosized hydroxyapatite powder doped with Mg ions (Mg-HAP) on the application of Mg-HAP sintered ceramics as dentin substitutes. The Mg-HAP powder was synthesized in the range of temperatures 150–180 °C, pressed into compacts and further sintered at 1200 °C. The physico-chemical and mechanical properties of obtained sintered ceramics, as well their bonding ability with commercially available dental restorative materials (composites, cements and adhesives) were tested.

The results showed that synthesis temperature does not influence the phasic composition of the obtained nanopowders, which were all shown to be monophasic hydroxyapatite. However, it did have influence on the phasic composition, densification, and mechanical properties of the sintered materials. The obtained Mg-HAP ceramics with controlled porosity were shown to have satisfactory mechanical properties (hardness by Vickers in the range 3.78–4.73 GPa, fracture toughness in the range 0.93–1.12 MPa·m^{1/2}) and adequate bonding ability with dental materials for application in restorative dentistry as dentin substitutes. Nevertheless, it was shown that even 10 °C difference in synthesis temperature of Mg-HAP powders influenced greatly the bonding ability of the dentin substitutes with the restorative

materials, due to the differences in phasic composition, solubility and mechanical properties.

O-3

INFLUENCE OF Yb³⁺ CONCENTRATION ON STRUCTURAL AND LUMINESCENT PROPERTIES OF Tm³⁺ DOPED SrGd₂O₄

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Here, samples of SrGd₂O₄ doped with different concentration of Yb³⁺ (2, 4, 6 at.%) ions and constant concentration of Tm³⁺ (1 at.%) were prepared. For preparation of samples, combustion method assisted with glycine as a fuel and citric acid as a chelator was chosen. All samples were heated in the furnace at 500 °C for 1.5 h and additionally thermally treated for 2.5 h at 1000 °C. X-ray diffraction (XRD) revealed that all peaks are assigned to the pure orthorhombic lattice of SrGd₂O₄, space group *Pnma* (JCPDS Card No.:01-072-6387). Field emission scanning electron microscopy (FE-SEM) showed agglomerated spherical particles with size around 150 nm. Energy dispersive spectroscopy confirmed uniform distribution of constitutive elements through the samples. Up-conversion emission properties were evaluated from photoluminescent emission spectra and intensity dependence on excitation power after excitation at 980 nm. Dominant blue emission with appropriate transition ¹G₄ → ³H₆ is detected in all samples, for which three photons are required.

O-4

CHARACTERIZATION OF ACTIVE CARBON MATERIALS OBTAINED FROM BIO WASTE FOR POTENTIAL USE IN WATER PURIFICATION

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Adsorption is one of the well-known methods in the removal of various pollutants from water bodies. The activated carbon material has great potential in water purification as an adsorbent. In process of adsorption various pollutants from water, such as different type of pathogens and toxins that can be potential risk for human health, can be effectively removed by activated carbon. The aim of this study is detail characterization of newly synthesized activated carbon materials from bio-waste. Dried date palm leaf stalk (*Phoenix dactylifera* L.) and black alder cone-like flowers (*Alnus glutinosa* L.) have been chosen as bio-waste precursors. The activated carbon materials were firstly carbonized in atmosphere of N₂ and then activated in atmosphere of CO₂. Both processes are performed at 750 °C during 1 h. The yields of materials were 36.5 % and 24.7 % made of datepalm leaf stalk (P_AC) and black alder cone-like (A_AC) flowers, respectively. The commercial activated carbon has been characterized in order to compare with synthesized materials. For structural and chemical properties of materials was characterized in detail by: X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), low temperature N₂ physisorption and Field emission scanning electron microscopy (FESEM). According to those results, materials obtained from date palm leaf stalk and black alder fruits show that newly synthesized materials have properties of an adsorbent with good potential for usage in water purification from different types of pollutants.

O-5

**BILAYER (La,Sr)MnO₃ AND (Ba,Sr)TiO₃ THIN FILMS
PREPARED BY CHEMICAL SOLUTION DEPOSITION
TECHNIQUES**

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Magnetoelectric (ME) effect is desirable property in spintronic and microelectronic devices. This effect occurs naturally in some single phase materials due the coexisting of ferroelectric and ferromagnetic order, but the intensity of this effect is not very useful in microelectronic applications. Artificial multiferroic composites are good alternative in which ME effect can be engineered and controlled by proper choice of interface geometry and constituent materials. The aim of this work was to create bilayer heterostructures in the form of thin epitaxial films in order to achieve good ME coupling through the magnetostrictive effect in the ferromagnetic layer and piezoelectric effect in the ferroelectric layer.

Bilayer heterostructures consisting of ferromagnetic La_{1-x}Sr_xMnO₃ (LSMO) and ferroelectric Ba_{1-x}Sr_xTiO₃ (BSTO) layers were deposited on Si and SrTiO₃ (001) substrates by spin-coating method. The bottom LSMO thin layer was obtained by polymer-assisted deposition (PAD) technique using aqueous solution of corresponding cations stabilized with PEI and EDTA additives. The BSTO layer was obtained by classical solution deposition method using BaCO₃, Sr(C₂H₄O₂)₂ and Ti-alcoxide. However, the influence of processing conditions on the formation of epitaxial BSTO thin film by PAD technique on the top of the LSMO layer was also investigated. Structural characterization of the obtained thin films was done by X-ray diffraction and HRTEM, while thickness and surface properties were determined by SEM and AFM. Measurements of electric and magnetic properties were also performed.

O-6

EPITAXIAL GROWTH OF LaMnO₃ THIN FILMS BY POLYMER ASSISTED DEPOSITION TECHNIQUE ON THE DIFFERENT MONOCRYSTALLINE SUBSTRATE

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Discovery of giant magnetoresistance (GMR), three decades ago is considered as a beginning of the new concept of electronic, known as a spintronic. Due to existence of GMR, lanthanum manganite materials are recognized as good potential candidates for development of completely new concept of magnetic memories based on the electronic spin. Specific application conditioned the development of LaMnO₃ based material in epitaxial thin film form. In last years, development of polymer assisted deposition (PAD) technique showed that solution deposition techniques have important place in fabrication of the highly oriented epitaxial thin films. One of the most important steps in epitaxial thin film preparation is selection of the substrate, which highly determines structure and properties of deposited layer.

In this study, PAD technique was used for production of polycrystalline and epitaxial LaMnO₃ thin films on the different substrates. Different concentrated solutions (from 0.1 to 0.5 M) of LaMnO₃ were prepared by dissolving of La(NO₃)₃·6H₂O and Mn(NO₃)₂·4H₂O in the distilled water, followed by addition of the water soluble polymers polyethyleneimine (PEI) and ethylenediamine tetraacetic acid (EDTA) which take part in solution stabilization. Prepared solutions were deposited by spin coating method on the previously cleaned silicon wafers and thermally treated at 700 °C in order to obtain polycrystalline LaMnO₃ thin films. After examinations of polycrystalline LaMnO₃ thin films, 0.1 M solution was selected for preparation of epitaxial films on the monocrystalline SrTiO₃ (110 and 001) and MgO (001) substrates. LaMnO₃ layer deposited on the substrates by spin coating method was thermally treated at the 750 °C and post annealed at the temperatures up to 900 °C. Post annealing treatment shows changes in thin films structure and helps to establish optimal temperature regime in order to obtain different LaMnO₃ phases.

O-7

ENERGY LANDSCAPE OF A RELAXED AMINO ACID, GLUTAMINE (L), ON TiO₂ SURFACES

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Linking inorganic systems with organic ones is a highly important avenue for finding new drugs and treatment methods. Tumor cells have an increased demand for amino acids due to their rapid proliferation, and several amino acids, such as Glutamine (L), have other roles in supporting cancer growth. One of the inorganic materials that can show antitumor properties is titanium dioxide and its crystal modification anatase has shown the highest surface reactivity. In this study we first locally optimized 2D-slab structures of undoped and Au/Ag/Cu doped anatase (001 and 101 surfaces), then similarly optimized a single molecule of Glutamine (L) in vacuum. Next, we placed the pre-optimized glutamine molecule in various orientations and on a variety of locations onto the relaxed substrate surfaces, and then performed *ab initio* relaxations of the molecule on the substrate slabs. We employed the DFT method with a GGA-PBE functional, as implemented in the Quantum Espresso code. Comparison of the optimized conformations and electronic structure of the amino acid in vacuum and on the surface, yield useful insights into various biological processes, while several physical interactions between molecule and surface (Figure 1) showed promising applications in biomedicine.

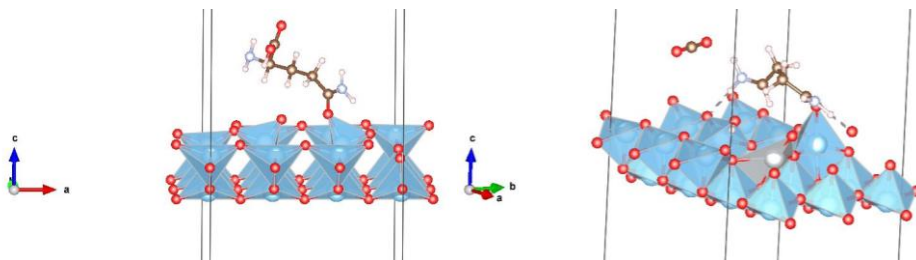


Figure 1. Optimized structure of Glutamine (L) molecule on: a) undoped anatase slab (001) surface; b) Ag doped anatase slab (001) surface, visualized by VESTA program

O-8

FIRST-PRINCIPLES INVESTIGATION AND STRUCTURE PREDICTION IN HOLMIUM(III) FLUORO-SELENIDE SYSTEM

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Ternary rare-earth metal compounds that contain fluorine and selenium (MFSe) crystallize into tetragonal PbFCl-type structures, with some orthorhombic, trigonal and hexagonal exceptions, and polytypes of MFSe also exist [1–3]. New modifications with different properties can also be found under different pressure and temperature conditions.

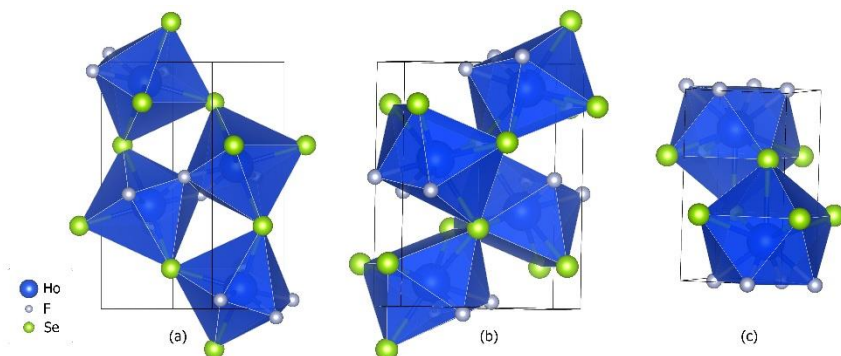


Figure 1. Calculated structures in the Holmium(III) Fluoro-Selenide system: a) α -HoFSe, orthorhombic $Pnma$ (no. 62); b) β -HoFSe, orthorhombic $Pnma$ (no. 62); c) γ -HoFSe, tetragonal $P4/nmm$ (no. 129).

In order to theoretically predict structure of new (and existing) stable and/or metastable modifications of HoFSe, the following methods were used. First, global exploration was performed on the energy landscape using simulated annealing with empirical potentials in G42+ software package [4]. Global optimization (GO) algorithm was applied to 4 fold (4 atoms of Ho, F and Se – 12 atoms in total) and 6 fold (6 atoms of Ho, F and Se – 18 atoms in total) formula units of HoFSe. Almost two million structure candidates were obtained this way. These structures were then symmetrized, grouped according to the space group to which they belong, and then compared using software package KPLOT [5] and the algorithm which we developed for this purpose. Structure type candidates were then sorted by relevance

criteria, such as ground state energy, number of structures found and symmetry. Eventually only a couple of hundred of relevant structure candidates remained. For them, local structural optimization was done on ab-initio level with different functionals (e.g. LDA, GGA-PBE and B3LYP) using CRYSTAL17 [6] software package. Some theoretically predicted structure candidates are shown in Figure 1.

Finally, $E(V)$ (energy vs. volume) and $H(p)$ (enthalpy vs. pressure) curves were calculated for chosen structure candidates in order to determine the stable phases at different pressures and the transition pressures.

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O-9

SYNTHESIS AND CHARACTERIZATION OF HAFNIUM CARBIDE BASED CERAMICS

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Two-dimensionally plain-woven polycrystalline SiC fiber cloth and yttrium doped HfO₂ nano-powders were used to fabricate the SiC-HfC ceramic composite via self-propagating high-temperature synthesis and simultaneous consolidation technique. The alternating layers of SiC and HfC were obtained by spark plasma sintering of stack of SiC cloths covered by electrophoretically deposited HfO₂. During sintering process, deposited HfO₂ was converted into HfC phase. The obtained composite material was characterized in terms of microstructure and cavitation resistance and oxidation resistance. The results show that spark plasma sintering technique is effective way to preserve fibre-like mikrostructure of SiC. The obtained composite ceramic showed good erosion resistance. During oxidation at high temperatures both carbides (SiC and HfC) form oxides (SiO₂ and HfO₂) that react and form a surface layer of hafnium silicate named hafnom that protects the silicon carbide from further oxidation. The weight gain confirmed the passive oxidation, i.e., the ability of formed oxide layer to prevent oxygen diffusion into the material.

O-10

EFFECT OF THE SINTERING TECHNIQUE ON THE PROPERTIES OF Sb-DOPED BaSnO₃ CERAMICS

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Barium stannate, BaSnO₃ (BSO), a cubic perovskite-type oxide with its interesting structural, optical and electrical properties has wide application as an electrode material, thermally stable capacitor, transparent conductive oxide, photocatalyst, humidity and gas sensor material [1]. Partial substitution of Sn by Sb in BSO leads to drastic changes primarily in its electrical properties, resulting in metallic-like conductivity of doped ceramics. Major problems concerning the synthesis of Sb doped BSO (BSSO) are connected to the phase composition and density of final ceramic material.

This study covers the comprehensive investigation of structural, microstructural and electrical properties of the Sb-doped BaSn_{1-x}Sb_xO₃ ($x = 0.00, 0.04$ and 0.08 , BSSO) ceramic materials obtained by two different sintering techniques: conventional sintering (CS) and Spark Plasma sintering (SPS). The relative densities of the BSSO-CS ceramic samples sintered at 1600 °C for 3 h was in the range of 79–96 %. On the other side, the relative densities of BSSO-SPS ceramic samples in the range of 86–96 % were obtained at 1200 °C, with sintering time of only 5 minutes.

The XRD analysis confirmed that cubic BaSnO₃ is a major phase in all BSSO samples. The presence of tetragonal Ba₂SnO₄ as a secondary phase was detected in BSSO-SPS ceramic samples, with its content decreasing upon Sb-doping. As expected, the grain size of the samples sintered at higher temperatures (BSSO-CS) is larger in comparison with BSSO-SPS ceramic samples, which was confirmed by Scanning Electron Microscopy (SEM). SEM analysis also revealed the layered structure within the grains of BaSn_{0.92}Sb_{0.08}O₃-CS sample while HRTEM analysis confirmed the existence of the low angle grain boundaries (LAGBs) in the SPSed sample with the same composition.

The electrical resistivity decreased upon Sb doping, and all doped BSSO samples showed the linear I - U characteristic in the temperature range of 25–150 °C. The semiconductor behavior of all BSSO-CS and BSSO-SPS ($x = 0.00$ and 0.04) ceramic samples was confirmed through the existence of semicircles in their impedance spectra. On the other hand, the BaSn_{0.92}Sb_{0.08}O₃ sample showed the metallic-like behavior resulting from the loss of the electrostatic barriers at LAGBs, which is manifested through the absence of the semicircle in its impedance spectra.

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P-1

SYNTHESIS AND STUDY OF CHROMIUM-DOPED DIOPSIDE CERAMIC PIGMENTS

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The aim of this study is to synthesize ceramic pigments based on stoichiometric diopside in the $\text{CaO} \cdot \text{Cr}_2\text{O}_3 \cdot \text{MgO} \cdot 2\text{SiO}_2$ system with different initial concentrations of chromium additives at four temperatures of sintering, as well as to study the change in phase composition and color.

Ceramic pigments are synthesized by solid-state high temperature sintering at 900, 1000, 1100 and 1200 °C in the system $\text{CaO} \cdot x\text{Cr}_2\text{O}_3 \cdot (1-x)\text{MgO} \cdot 2\text{SiO}_2$, where $x = 0.1, 0.2, 0.3, 0.4$ and 0.5 . The starting materials used for the synthesis are CaCO_3 , Cr_2O_3 , MgO and $\text{SiO}_2 \cdot n\text{H}_2\text{O}$. Calculated quantities of materials for 100 g batch are weighed, mixed and homogenized in planetary mill. The synthesis is performed in a laboratory muffle furnace in porcelain crucibles with a heating rate of 300–400 °C/h in air with isothermal retention of 2 h at final temperature.

The obtained ceramic pigments were examined by powder X-ray diffraction analysis, electron scanning microscopy, infrared, UV-Vis and EPR spectroscopy. It has been established that multiphase ceramics are obtained under synthesis conditions. The main mineral phases are diopside - $\text{MgCaSi}_2\text{O}_6$, spinel - MgCr_2O_4 and wollastonite - CaSiO_3 . The color of the resulting ceramics is green. The effect of chromium concentration and sintering temperature on phase composition and color was studied.

At 1000 °C polyphase ceramic that contains diopside, Mg chromite -spinel MgCr_2O_4 , and wollastonite is obtained. At low concentration of Cr (Cr = 0.1 and 0.2) diopside and chromite are prevailing phases nonreacted MgO is separated as periclase. The concomitant phase is wollastonite. At higher concentration of Cr (Cr ≥ 0.3) Cr_2O_3 is separated. It is seen that high concentration of chromium suppresses the formation of diopside.

The results of the measurement of the color coordinates show that as the firing temperature increases, the color of the pigments changes from gry to green. As the firing temperature increases, there is a tendency for the brightness L^* to increase, and the coordinates a^* and b^* decrease their values. The amount of green color ($-a^*$) is greatest in the ceramics sintered at lower temperature (1100 °C).

The synthesized pigments are suitable and can be successfully applied in glaze tiles and sanitary ceramics.

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P-2

STUDY OF CERAMIC PIGMENTS IN THE SYSTEM $\text{CaO} \cdot x(\text{REE}) \cdot (1-x)\text{MgO} \cdot 2\text{SiO}_2$

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Ceramic pigments are synthesized via solid-state high temperature sintering at 900, 1000, 1100 and 1200 °C in the system $\text{CaO} \cdot x\text{Pr}_2\text{O}_3 \cdot (1-x)\text{MgO} \cdot 2\text{SiO}_2$ and $\text{CaO} \cdot x\text{Er}_2\text{O}_3 \cdot (1-x)\text{MgO} \cdot 2\text{SiO}_2$, where $x = 0.1, 0.2, 0.3$. Starting materials used for the synthesis are CaCO_3 , Pr_6O_{11} , Er_2O_3 , MgO and $\text{SiO}_2 \cdot n\text{H}_2\text{O}$ with particle size in the range of 2–7 μm , which is much more reactive than conventionally used quartz sand as a source of SiO_2 . Calculated quantities of materials for 100 g batch are weighed, mixed and homogenized in planetary mill Pulverizete-6 (Fritch). Synthesis was carried out in a laboratory muffle furnace in porcelain crucibles with a heating rate of 300–400 °C/h in air with isothermal retention of 2 h at the final temperature.

The obtained ceramics were examined by powder X-ray diffraction analysis, electron scanning microscopy, infrared and UV-Vis spectroscopy. It has been found that under synthesis conditions a multiphase ceramics is obtained. The colors of the ceramics are gray and light pink. The effect of praseodymium and erbium concentration and sintering temperature on the phase composition and color was studied.

The main mineral phases in erbium doped ceramics are diopside, wollastonite, äkermanite and periclase. At low temperatures (900 and 1000 °C) merwinite is formed, which disappears at temperatures above 1100 °C, where the rare earth silicate $\text{Ca}_2\text{Er}_8(\text{SiO}_4)_6\text{O}_2$ with apatite-type of crystal structure appears. Excess of SiO_2 is separated as cristobalite.

The main mineral phases in Pr-doped ceramics are $\text{Ca}_2\text{Pr}_8(\text{SiO}_4)_6\text{O}_2$ and praseodymium oxide. At low temperatures (900 °C) merwinite and äkermanite are formed, while the diopside crystallizes above 1100 °C only as an additional phase.

It was found that the addition of rare earth oxides to this composition does not favor the formation of diopside ceramics.

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P-3

STRUCTURAL AND CHEMICAL PROPERTIES OF WASTE VITREOUS ENAMELS GENERATED DURING THE PRODUCTION PROCESS OF HEATING DEVICES

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The subject of this research is to ensure the most efficient use of resources in the process of manufacturing heating devices, all with the aim of the concept of cleaner production. Waste vitreous enamels have significant potential and usability and with appropriate physical and chemical properties can be applied in the construction industry. For that purpose, waste vitreous enamel was firstly characterized in detail by X-ray powder diffraction (XRD), diffuse reflectance infrared Fourier transform spectroscopy (DRIFT) and field emission scanning electron microscopy (FESEM), while the chemical analysis and determination of the content of heavy metals were performed using inductively coupled plasma optical emission spectrometry (ICP-OES). Based on the qualitative mineralogical analyzes, it was found that quartz is the most represented mineral in both groups of samples, while the oxides of metals Sb, Fe, Ti, Cu appear in the form of supporting minerals are senarmontite, hematite, rutile and tenorite. The strong band at 958 cm^{-1} confirmed characteristic bands of Si–O and O–Si–O group and indicated the presence of the silicate minerals. FESEM analysis revealed that waste materials show large particles, bimodal particle distribution and small porosity. Obtained results indicate the possibility that waste vitreous enamels from the production process can be used in mortar and concrete production as a partial cement replacement with a minimal negative impact on the environment and at the same time solve the problem of its disposal.

P-4

**CHARACTERIZATION OF HIGH TEMPERATURE CERAMIC
COMPOSITE SEALANTS (CCS) WITH ADDITION OF
ALUMOSILICATE BASED WASTE MATERIAL FOR THE
POTENTIAL USE IN IT-SOFC**

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In the present paper, possible application of novel concept synthesis method of ceramic composite sealants (CCS) with implementation of aluminosilicate-based waste material in intermediate temperature solid oxide fuel cells (IT-SOFC) was investigated. Besides two different basic variants of alumina matrix nanocomposites stabilized by rare earths and carbon materials (CCS-RE and CCS-C), for this purpose two additional sealant compositions with 5 wt.% addition of waste material (CCS-RE5 and CCS-C5) were designated for a comparative study.

The aim of this research was to characterize the waste material, as well as the starting components used for developing ceramic composites through various characterization techniques. Analytical procedures for determining chemical composition with focus on heavy metal content in waste was performed in order to ensure the waste is ecologically acceptable to be used as an additive. Besides, the crystalline phase composition of the raw materials as well as of the sealant compositions was determined by X-ray diffraction (XRD) analysis.

Finally, obtained results revealed that this research may provide the possible solution of forming a cost-effective, environmentally-friendly and high-efficient ceramic sealants for application in IT-SOFC by incorporating waste materials in its composition, without significant negative effects on its performance and main properties.

P-5

SURFACE MODIFICATION OF CeO₂ NANO-POWDER

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A wide range of visible-light-responsive organic/inorganic surface complexes between CeO₂ nano-powder and salicylate- and catecholate-type of ligands were synthesized for the first time. Surface modification of CeO₂ nano-powder, synthesized by a self-propagating room temperature method with salicylate-type of ligands (salicylic acid and 5-aminosalicylic acid) as well as catecholate-type of ligands (catechol, 3,4-dihydroxybenzoic acid, caffeic acid and 2,3-dihydroxy naphthalene) induces the appearance of absorption in the visible spectral region due to interfacial charge transfer (ICT) complex formation. Their optical properties were thoroughly analyzed by experimental and theoretical methods. Thorough characterization involving transmission electron microscopy, XRD analysis, and nitrogen adsorption-desorption isotherms, revealed that loosely agglomerated CeO₂ particles in the size range from 2 to 4 nm. The attachment of salicylate- and catecholate-type of ligands to the surface of CeO₂ powders lead to the formation of colored powders with tunable absorption in the visible spectral region. The density functional theory calculations with properly design model systems were performed in order to estimate the energy gaps of various inorganic/organic hybrids.

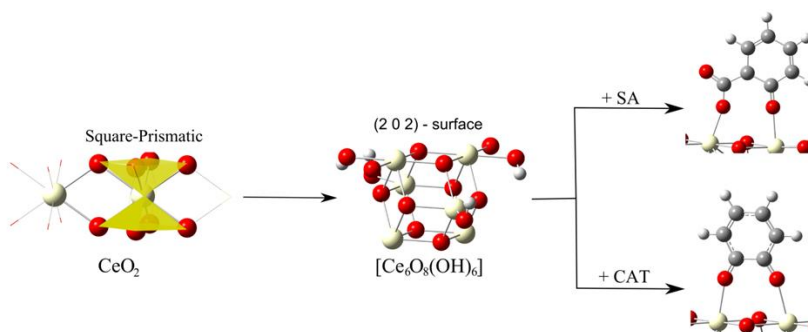


Figure 1. The square-prismatic coordination of Ce⁴⁺ ions in the crystal structure of cubic CeO₂ (P₁ – space group), the cluster that has been constructed based on the (2 0 2) crystal plane, and the bidentate coordination mode of salicylate- and catecholate-type of ligands.

P-6

**SYNTHESIS OF OBTAINING SiO₂ FROM BIOMASS,
CHARACTERIZATION OF STRUCTURAL AND CHEMICAL
PROPERTIES AND THE POSSIBILITY OF POTENTIAL
APPLICATION**

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The main goal of this research is to obtain carbon material (by pyrolysis of biomass in the presence of inert gas N₂) and then physical activation with CO₂ obtained active carbon material and finally chemical treatment (using TEOS - tetraethyl orthosilicate) enabled the creation of highly porous bio-SiO₂ ceramics. The results of experiments of pyrolysis at several high operating temperatures, activation of carbon material and with multicycle action using TEOS clearly showed the possibility of obtaining SiO₂ nanostructures, after carbothermal reduction to 600 °C. Increasing the activation temperature and the duration of the activation process initiates the development of SiO₂ particles within the porous structure. The final SiO₂ powder product was analyzed by several different test methods. Structure and morphology were analyzed by X-ray diffraction (XRD) and scanning electron microscope (SEM). Surface chemistry and functional surface groups were determined by Fourier Transform Infrared Spectroscopy (FTIR).

The obtained results are guidelines for further study and understanding of the properties of SiO₂ and for the possibility of its application

P-7

HIERARCHICAL ZnO/SnO₂ HETEROSTRUCTURES VIA HYDROTHERMALLY ASSISTED ELECTROSPINNING TECHNIQUE: SYNTHESIS AND PHOTOCATALYTIC PERFORMANCES

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Hierarchical nanostructures with multiporous tin oxide nanofibers (SnO₂-MPNFs) and zinc oxide nanorods (ZnO-NRs) have been synthesized by combining electrospinning technique and hydrothermal method. A solution containing uniformly distributed tin (Sn) and silicon (Si) species of precursors, as well as a sacrificial polymer (PVP) was electrospun using a single-nozzle spinneret to fabricate nanofibers. In virtue of the Kirkendall effect driven by calcination at 550 °C, the SiO₂-cored SnO₂ nanofibers (SnO₂-SiO₂-NFs) deliberated from PVP were formed and used as backbones for further hydrothermal growth of ZnO-NRs. By varying the hydrothermal reaction time (0.5–2 h) at the constant concentration of SnO₂-SiO₂-NFs, zinc (Zn) precursor, directing agent (hexamethylenetetramine, HMT) and aqueous ammonia, the density, length and thickness of ZnO-NRs were controlled. Nanofibers and ZnO-NRs/SnO₂-MPNFs heterostructures are confirmed by X-ray diffraction (XRD), field-emission scanning electron microscopy (FE-SEM), energy dispersive spectrometer (EDS), transmission electron microscopy (TEM) and elemental mapping analysis.

The hydrothermal treatment conducted at 90 °C in aqueous ammonia allowed: a) selective etching of SiO₂ from the SnO₂-SiO₂-NFs core and SiO₂ trapped between SnO₂ particles, and b) effective growth of ZnO-NRs. The process resulted in ZnO-NRs/SnO₂-MPNFs heterostructures with ZnO-NRs of 1–5 μm in length attached to SnO₂-MPNFs, the shell of which was composed of ultra-fine SnO₂ crystallites (~5 nm in size) and where the four porous channels create the core instead of SiO₂. Photocatalytic performance of the heterostructures was investigated toward different organic azo-dyes (methylene blue, methyl orange) and obvious enhancement was demonstrated in degradation of the organic pollutant, compared to primary SnO₂-based nanofibers.

P-8

XANTHATE ABSORPTION KINETICS AS A FUNCTION OF THE STARTING CONCENTRATION WITH THE USE OF THE WASTE SLAG AS ADSORBENT

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In order to avoid environmental issues considering disposal of great volumes of waste generated from the mining industry processes there is a tendency among researchers to find potential use of these harmful by-products. Waste slag is one such waste product since the content of different undesirable elements like cadmium, arsenic, zinc and other heavy metals may be at a level that can potentially endanger the environment and cause public health issues.

On the other hand, tailings generated in the flotation facilities are also considered to be environmentally harmful because of different residual organic reagents that are applied in the process. As it is well-known, xanthates are the most widely used reagents in flotation processing of the sulfide ores, and, therefore largely present in tailings. Besides, xanthates are reported to pose toxicity and numerous negative impacts from the ecological point of view. That explains why it is of great importance to find efficient and low-cost routes for minimizing their remaining levels in tailings, therefore exposure to environment.

In this study, xanthate absorption by using of the waste slag as adsorbent was investigated. For that purpose, three different starting concentrations of xanthates were selected, -20, 50 and 90 mg/l. The mass of the adsorbent i.e. waste slag put into 50 ml of xanthate solution amounted to 0.01 g. Experiment was conducted on room temperature while pH value was set to be 10. The percentage of the total xanthates content absorbed was evaluated after the period of 24 h. Obtained results indicated that potential reuse of the waste slag for the removal of xanthates, may be justified and after 24 h, 98 %, 58 % and 62 % of the xanthates were adsorbed, respectively. However, further examination is needed in terms of better understanding of xanthate absorption mechanisms and improvement of waste slag absorption efficiency.

P-9

BEHAVIOUR OF Mg AND Si SUBSTITUTED HYDROXYAPATITES IN MODEL MEDIA

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Thanks to its similarity with biological apatite found in vertebrate hard tissues, calcium hydroxyapatite is one of the most investigated materials in bone tissue engineering. Since biological apatite is not stoichiometric, ion substituted hydroxyapatites are in the focus of many studies as they more closely mimic the composition of natural bone. Although there are many investigations of the influence of foreign ions on the structure and physico-chemical properties of ion-substituted hydroxyapatites, there is no much information on their behaviour in different media.

In present study, magnesium - which plays a key role in bone metabolism and silicon - which is necessary for normal skeletal development, were used as ion substitutes. The behaviour of Mg and Si substituted hydroxyapatite in simulated body fluid and physiological solution was investigated by XRD, FTIR and SEM. Obtained results confirmed great potential of these substituted hydroxyapatites for biomedical applications.

P-10

**IMPROVED PHOTOCATALYTIC DEGRADATION OF RO16
DYE USING HYDROTHERMALLY SYNTHESIZED CeO₂@ZnO
NANOCOMPOSITE**

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The structural, microstructural, optical and photocatalytic properties of hydrothermally obtained single-phase ZnO and CeO₂@ZnO nanocomposites have been investigated by the XRPD, FESEM, HRTEM/SAED and UV-vis techniques. In order to improve the photocatalytic efficiency of ZnO, the optimal CeO₂ content in ZnO powders was determined by varying the quantity of CeO₂ from 0 to 10 mol%. The results showed that CeO₂ with spherical crystallites of about 5 nm was distributed onto the ZnO surface, whose crystallites displayed a bimodal distribution, from nano- to microcrystallites. The morphology of ZnO particles varied from elongated nanograins to microrods that further formed a 3-D tie-like morphology which was disrupted by CeO₂ adding. By degrading 90% of RO16 dye in 180 minutes, the composite containing 5 mol% of CeO₂ showed approximately for 30% better photocatalytic efficiency comparing to other samples, although all the obtained powders have similar structural, microstructural and optical characteristics. This is obviously the optimal ratio of these two phases, in which synergy of CeO₂ adsorption and ZnO photocatalytic effect reaches its maximum due to reduced recombination rate and improved adsorption. The kinetic of RO16 degradation could be described by a pseudo-first order model.

P-11

VISIBLE-LIGHT PHOTOCATALYTIC DEGRADATION OF MORDANT BLUE 9 BY BiVO₄ NANOPOWDER

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CaMnO₃-based ceramics doped with gadolinium has become a matter of great scientific interest, because of their physical, electronic and magnetic properties, and many intriguing phenomena, such as colossal magnetoresistance (CMR) involving potential applications in magnetic memory devices and sensors. Electronic properties of CaMnO₃ doped with different amount of gadolinium were investigated using combination of experimental and theoretical methods. Spectroscopic Ellipsometry has been used to study electronic properties and band gap variation as function of Gd doping (up to 20% Gd). Furthermore, for each of the structure candidates, a local optimization on the *ab initio* level using density-functional theory (DFT), hybrid (B3LYP) and the Hartree–Fock (HF) method was performed.

P-12

INVESTIGATING SORPTIVE ASPECTS OF CoMoO₄ NANOPOWDERS SYNTHESIZED BY SPRT METHOD

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Nanosized CoMoO₄ solid solution was successfully synthesized at room temperature using simple and fast Self Propagating Room Temperature procedure (SPRT). The structural, textural, morphological and surface characteristics of the nanosized CoMoO₄ were examined in detail by X-ray diffraction (XRD), Fourier transform infrared (FT-IR) spectra, Field emission scanning electron microscopy

(FESEM), and nitrogen sorption method. X-ray powder diffraction (XRPD) reflected the presence of two different phases that are in the same space group. The α -CoMoO₄ and the β -CoMoO₄ modification crystallizes in the monoclinic space group *C2/m*, No.12, but the β -phase clearly distinct from the α -phase due to the tetrahedral coordination of the Mo⁶⁺ ions. Adsorption tests were studied over CoMoO₄ nanopowders under different experimental conditions (material dosage, initial concentration of pollutant textile dye, etc). The obtained results showed acceptable sorption characteristics of the material.

1. D. Zagorac, J.C. Schön, M. Rosić, J. Zagorac, D. Jordanov, J. Luković, B. Matović, *Crystal Res. Technol.*, **52** [10] (2017) 1700069.

P-13

ION MIGRATION IN SPINEL STRUCTURE IN NICKEL AND ZINC FERRITE NANOPOWDERS SYNTHESISED BY CO-PRECIPIATION AND HYDROTHERMAL METHODS

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Nickel and zinc ferrite systems were synthesized as single phase materials, core/shell composites and mixed ferrite phase using co-precipitation and hydrothermal methods. Evolution of spinel structure and degree of inversion were followed by using XRD and Raman spectroscopy. Rietveld refinement was used to evaluate crystal structure parameters and phase composition. Deconvolution of Raman spectra was used in order to determine cation coordination and degree of inversion. It was established that both zinc and nickel ferrite showed mixed ferrite characteristics which is in contrast with their bulk structures. TEM micrographs confirmed formation of core/shell particles with distinct nickel ferrite core and zinc ferrite shell with the sizes of about 100 nm.

P-14

**STABILITY AND FUNCTIONALITY OF $\text{BaCe}_{1-x}\text{In}_x\text{O}_{3-\delta}$ AS A
HIGH TEMPERATURE PROTON CONDUCTING
ELECTROLYTE FOR SOLID OXIDE FUEL CELLS**

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Mixed oxides with the perovskite structure are known for their proton conducting ability at the temperatures above 500 °C. This characteristic makes them suitable for application as an electrolyte for intermediate-temperature solid oxide fuel cells. Doping of BaCeO_3 with In^{3+} in place of Ce^{4+} leads to emergence of oxygen vacancies which take part in creation of proton defects.

The characteristics of the $\text{BaCe}_{1-x}\text{In}_x\text{O}_{3-\delta}$ were investigated in a wide range of In dopant concentrations ($x = 0.05; 0.10; 0.15; 0.20; 0.25; 0.30; 0.35$ and 0.40). All the samples were synthesized by a citric-nitric autocombustion method. The dense electrolytes were formed after sintering at 1300 °C for 5 h in air. X-ray powder diffraction analysis showed that powders with In content greater than 25 mol% contained In_2O_3 as a secondary phase. The highest total conductivity around $5 \times 10^{-3} \text{ S} \cdot \text{cm}^{-1}$ was measured for the sample $\text{BaCe}_{0.75}\text{In}_{0.25}\text{O}_{3-\delta}$ in the wet hydrogen atmosphere at 700 °C. After exposure to pure CO_2 atmosphere at 700 °C for 5 h, the samples were investigated by X-ray diffraction analysis. It was found that even 15 mol% In could completely suppress degradation of the electrolyte. Ni- $\text{BaCe}_{0.75}\text{In}_{0.25}\text{O}_{3-\delta}$ / $\text{BaCe}_{0.75}\text{In}_{0.25}\text{O}_{3-\delta}$ /LSCF- $\text{BaCe}_{0.75}\text{In}_{0.25}\text{O}_{3-\delta}$ fuel cell was tested in wet hydrogen atmosphere and power density output of $264 \text{ mW} \cdot \text{cm}^{-2}$ was measured at 700 °C. This result is an indication of stability and functionality of this electrolyte and its versatility in respect to type of fuel and performing environment.

P-15

ENHANCED PHOTOCATALYTIC REMOVAL OF CONGO RED BY MOF-ACTIVATED CARBON COMPOSITE

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Rapid industrialization and increasing population have increased the water demand. Various wastes from industries and anthropogenic activities are discharged into aquatic bodies such as lakes, ponds, rivers, oceans. Therefore, focus is placed on the removal of the contamination from the wastewater.

Organic pollutants gained extensive attention because of their toxicity, persistence and significant impacts on human health. Among them, organic dyes are complex molecules and most of them are water-soluble, resistant to detergents and heat, exhibit poor biodegradability, etc. Azo dyes are used in about 70% of commercial dyes today, from textile and plastic to cosmetics and food.

In this work, removal of azo-type dye Congo Red (CR) from water was performed by using UiO-66 type MOF (Metal Organic Framework), activated carbon (AC) and their composite powder mixture (MOF/AC = 50/50 wt.%). Samples were exposed to solar light irradiation for 1h and 2.5 h, respectively, centrifuged to remove solid particles, and solutions were analyzed by UV-ViS spectrophotometer in order to determine the concentration of the remaining dye. Process was repeated three times in order to explore the renewability of the photocatalysts used, with catalysts dried at 50 °C between cycles. Results revealed superior photocatalytic cycling performance of the MOF compared to the MOF/AC composite, while AC showed decline in dye removal performance due to the saturation of available adsorption sites. MOF/AC composite exhibited beneficial cost/performance ratio.

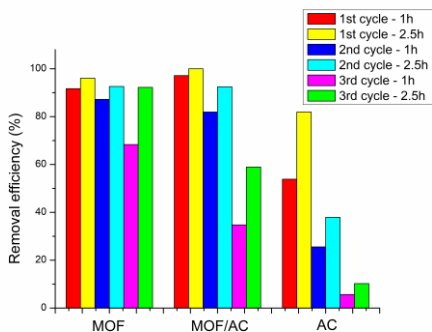


Figure 1. Removal of the CR from the water by using three different catalysts

P-16

COMPETITIVE REMOVAL OF DIVALENT HEAVY METAL IONS FROM SYNTHETIC AND REAL WASTEWATER BY ARAGONITE SEASHELL WASTE

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For industrial wastewater treatment, especially when it comes to effluents with high metal concentrations (>1000 mg/L) and low pH, limestone and lime are commonly used materials. In order to reduce the exploitation of natural limestone deposits, various biogenic waste materials are investigated as sustainable alternatives. Seashell waste, often accumulated in coastal areas due to harvesting and farming various seashell species for human consumption, is a source of biogenic calcium carbonate and shows potential in neutralization and metal immobilization processes. For practical use, knowledge of the effects of competition among pollutants for the sorbent's limited capacity is essential given the complex composition of metal-bearing effluents.

This study presents the applicability of aragonite-based seashell waste powder (SW) in the concurrent removal of heavy metals from synthetic and industrial wastewater. Synthetic solutions were prepared as a series of equimolar mixtures of divalent heavy metals (Pb, Zn, Cu, Sr) with a wide range of total concentrations and a constant initial pH of 5.0. On the other hand, industrial wastewater collected at the Mining and smelting complex (Bor, Serbia) was characterized by high acidity (pH 1.6) and Cu, Zn, Fe, Ni, and Pb in concentrations ranging from a few mg/L to several hundred mg/L. The experiments were performed under batch conditions, mixing SW with liquid phases and measuring metal concentration and pH values before and after treatment.

The shapes of the constructed sorption isotherms and maximum sorption capacities of metals in model mixtures differed significantly with respect to data obtained in single-component systems. The effect of ion competition led to a decrease in the removal of all metals and simultaneously changed the SW selectivity towards investigated cations. The dominant removal of Pb from the mixture was explained by the low solubility product of cerussite identified in the residue. Results indicate that at high metals concentrations, the precipitation of metal carbonate with the lowest solubility product may passivate the SW surface and suppress the removal of other cations in the mixture. Therefore, in experiments with real wastewater, the dose and granulation of SW were varied, and it was shown that high removal rates of all pollutants could be achieved by optimizing these factors. Furthermore, calcination of SW at 900 °C completely transformed aragonite to CaO, which alkaline reaction led to precipitation of metal hydroxides from wastewater, enabling

efficient treatment at lower doses compared to untreated SW. Accordingly, the seashell waste powder may substitute limestone and lime in treating various metal-bearing wastewaters, especially in regions where it is available in large quantities.

P-17

THE USE OF MANGANESE(II)–PYROMELLITATE COMPLEX PRECURSOR FOR THE SYNTHESIS OF NANOSIZED MANGANESE OXIDES

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The increasing interest for nanosized mixed metal oxides such as spinels and spinel-based materials in last decades has been motivated by their wide applications in photocatalysis, magnetism or solar cells [1]. So far, those materials have been obtained by conventional ceramic routes that involved high temperature treatments of precursors like mixed nitrates, carbonates or hydroxides [1]. An approach based on thermal degradation of metal-organic coordination compounds has been found as a promising for the preparation of fine-dispersed spinel and spinel-based oxides, mostly because of the control over stoichiometry as well as the possibility to obtain the materials with the homogeneous distribution of metal ions [1].

As a continuation of our research relating to the design and synthesis of metal-organic coordination compounds with the aim of obtaining possibly new functional materials [2], herein we present the synthesis and characterization of new Mn(II)–dipyridylamine coordination compound with tetraanion of 1,2,4,5-benzenetetracarboxylic (pyromellitic) acid. The complex was used as a single-source precursor for the preparation of nanosized Mn₂O₃/Mn₃O₄, Mn₂O₃ and Mn₃O₄ by direct thermolysis in air atmosphere at 450, 965 and 1200 °C, respectively. The main goal of this research was to investigate the influence of decomposition temperature of the precursor on stoichiometry of the resulting nanocrystalline spinel-based manganese oxides. The structural, morphological and spectroscopic properties of these ceramic materials were also investigated.

1. H. Lu, D.S. Wright, S.D. Pike, *Chemi. Commun.*, **56** (2020) 854.
2. L. Radovanović, J. Zdravković, B. Simović, Ž. Radovanović, K. Mihajlovski, M. Dramićanin, J. Rogan, *J. Serbian Chem. Soc.*, **85** (2020) 1475.

P-18

**SURFACE CHARACTERIZATION AND PHOTOCATALYTIC
ACTIVITY OF NEWLY SYNTHESIZED Dy DOPED SrGd₂O₄
PHOSPHORUS**

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In this study, we present surface examination and investigation of the photocatalytic activity of a newly synthesized down-conversion luminescent nanomaterial SrGd₂O₄ doped with Dy³⁺ ions. Samples were prepared *via* glycine-assisted combustion method, were formed gel was firstly burned at 500 °C for 1.5 h and then calcined at 1000 °C for 2.5 h. To see the crystallinity and phase purity, X-ray diffraction (XRD) measurements were performed and showed that doped sample crystallizes as a single phase with the orthorhombic lattice of SrGd₂O₄. Luminescent characterization indicated presence of all appropriate emission peaks related to Dy³⁺ dopant ions. X-ray photoelectron spectroscopy (XPS) was used to investigate surface composition and survey spectra confirmed presence of expected elements (Sr, Gd, O and Dy). Photocatalytic properties of SrGd₂O₄:Dy were explored in the photocatalytic degradation of organic dye methyl orange (MO) under simulated solar light irradiation. UV/Vis spectrometer was used to measure a decrease in MO concentration in water solutions during the experiment. Aliquots of the working solutions were taken at the exact time intervals, and the results indicate successful dye decomposition rate after 4 h.

P-19

THE EFFECT OF TEMPERATURE ON THE SORPTION OF LEAD ON NATURAL BENTONITES

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Environmental pollution by lead (Pb(II)) has become an important issue due to its harmful effects on human health and environment. In this study, the effect of temperature on the sorption of Pb(II) from aqueous solutions on natural Slovak bentonites from three localities (Jelšový Potok, Lieskovec, and Hliník and Hronom) was investigated. All experiments were carried out under batch processing conditions, with the amount of sorbent, initial pH, initial concentration of Pb(II) and temperature as the variables. The degree of metal adsorption was evaluated analyzing the samples by atomic absorption spectrometry before and after adsorption.

The results showed that the adsorption of Pb(II) by bentonite samples is a rapid reaction process, and the adsorption capacity of bentonite from Jelšový Potok is significantly greater than the other two bentonite samples. The Langmuir, Freundlich, Elovich and Tempkin isotherm models were tried to represent the equilibrium data of Pb(II) adsorption. The adsorption data was fitted very well to the Langmuir isotherm model in the studied concentration range of adsorption. The Langmuir maximum adsorption capacities of the used bentonite samples were calculated. Isotherms have been used to determine thermodynamic parameters of the process: free energy change (ΔG°), enthalpy change (ΔH°) and entropy change (ΔS°). The effect of temperature was investigated in the temperature range from 293 K to 313 K. The calculated values of thermodynamic factors demonstrate that the process of adsorption is endothermic, spontaneous as well as feasible in nature.

These results indicated that the natural bentonite from Jelšový Potok had the best sorption properties from bentonites we used in this study for the removal of Pb(II) from synthetically prepared solutions.

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P-20

**THE CATALYTIC DEGRADATION OF RO16 DYE UNDER
DARK AMBIENT CONDITIONS USING
La-Ni-Nb-O-BASED POWDERS**

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Dyes released from textile industries present a big threat to the environment, and remediation of wastewaters became one of the major scientific challenges. In recent years, there has been a great need for catalysts that would oxidize pollutants under dark ambient conditions without the use of external stimulants like light, temperature, or additional chemicals such as O₃, H₂O₂. Efficient work of these catalysts would significantly reduce the energy consumption. Among other materials, perovskite-type oxides with general formula ABO₃ emerged as possible catalysts for dye degradation in the dark conditions. Lanthanum nickelates with single (LaNiO₃) and layered perovskite structure (La₄Ni₃O₁₀, La₃Ni₂O₇, La₂NiO₄) showed good catalytic properties, due to the existence of nickel in two oxidation states (Ni²⁺ and Ni³⁺) and the oxygen non-stoichiometry in these materials [1].

This study presents structural, microstructural and catalytic properties of the LaNi_{1-x}Nb_xO₃-based (xNb = 0.000, 0,005 and 0,010; La-Ni-Nb-O) powders prepared by mechanical activation method. The XRD (X-Ray Diffraction) analysis revealed the existence of a multiphase oxide system, including layered structures of nickelates La_{n+1}Ni_nO_{3n+1} (n = 3, 2, 1, 0) and NiO phase in all La-Ni-Nb-O-based powders. Also, the HRTEM (High Resolution Transmission Electron Microscopy) analysis confirmed the presence of structural polytypes in these powders. The catalytic properties of La-Ni-Nb-O-based powders were investigated by degradation of the anionic azo dye, Reactive Orange 16 (RO16), under dark ambient conditions at different pH values (3, 6.5, 9.5 and 11) and temperature of 20 °C. The best catalytic efficiency in the degradation of RO16 dye showed the sample with x(Nb) = 0.010 in acidic solution, where the residual of RO16 dye was about 4.5 % after 330 minutes. The reusability test for this powder in degradation process of RO16 dye showed that the sample with x(Nb) = 0.010 retained its catalytic activity during three cycles.

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P-21

ULTRASONIC SYNTHESIS AND CHARACTERIZATION OF MESOPOROUS MONOCLINIC BiVO₄ NANOPOWDER

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The BiVO₄ sample was successfully synthesized from a mixture of ammonium vanadate, bismuth(III) nitrate, and nitric acid exposed to ultrasound irradiation. Structure, microstructure and optical properties of the obtained BiVO₄ nanopowder were investigated. X-ray diffraction (XRD) analysis confirmed single phase monoclinic lattice system with average crystallite size of 50 nm in diameter. Scanning electron microscopy (SEM) micrographs revealed the tendency of crystallites to agglomerate forming larger irregular sub-micron spheres. Brunauer-Emmett-Teller (BET) method was used to estimate the specific surface area of the sample and determine pore shape and size. UV-vis spectroscopy measurements have revealed favorably high absorbance of the visible light with the calculated band-gap value of 2.48 eV. Calculated values of valence and conducting band energies are +2.77 eV and +0.29 eV respectively, suggested that BiVO₄ can be used for photocatalytic degradation under sunlight irradiation as evident from the UV-vis spectrum.

P-22

BLUEBERRY WINE BIOLOGICALLY ACTIVE COMPOUNDS PROTECT AGAINST OXIDATIVE STRESS

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Fruit and derived product represent a rich source of biologically active compounds which exhibit beneficial health effect on human organism. Among fruit especially berries it is important to highlight blueberries. One of derived products with added value from this fruit is wine. The aim of this study was to investigate *in vitro* activity of blueberry wine by monitoring activities of antioxidant protection enzymes and lipid peroxidation (malondialdehyde level) in isolated rat synaptosomes. Fruit wines were produced in controlled conditions of different microvinifications in which pure culture of selected wine yeast was used. Synaptosomes were isolated from the brain of Wistar albino rats. Analyzed wine samples influenced on the activity of antioxidant protection enzymes. Wine samples also showed ability to decrease malondialdehyde level. Activity for superoxide dismutase in synaptosomes was in range (6.47–7.21 U/mg) while catalase activity was (0.045–0.061 U/mg). Glutathione peroxidase activity was in range (0.0212–0.0232 U/mg), as well as malondialdehyde level (2.17–2.35 nmol/mg). Obtained results indicate that blueberry wines possess antioxidant properties and abilities to protect against free radicals generated during oxidative stress.

P-23

**HYDROTHERMAL SYNTHESIS, CHARACTERIZATION AND
APPLICATION OF ACTIVATED CARBON MATERIALS
OBTAINED FROM SACCHARIDES**

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In presented work, influence of temperature, starting material concentration and different hydroxides on properties and morphology of activated carbon obtained from saccharose were investigated. The samples were prepared by hydrothermal treatment and activated using KOH, NaOH and LiOH. Two saccharose concentrations (0.5, 1.0 mol/dm³) and three different temperatures (160, 200, 240 °C) were changed in hydrothermal treatment. Activation processes were performed at 750 °C under inert atmosphere. Obtained samples were characterized by X-ray powder diffractometry, elemental analysis, N₂ adsorption-desorption measurements, Fourier-transform infrared spectrometry, scanning electron microscopy and thermal analysis. The obtained samples were tested for potential application in dyes removal (Methylene Blue and Methyl Orange) from water solutions.

P-24

**WHAT COULD BE THE REASON FOR DIFFERENT BEHAVIOR
OF PHOSPHATE TUNGSTEN AND PHOSPHATE
MOLYBDENUM BRONZES IN BRIGGS-RAUSCHER
REACTION: NEW INSIGHT**

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Recently, two different effects of phosphate tungsten (PWB) and phosphate molybdenum (PMoB) bronzes (obtained by thermal treatment), on oscillatory Briggs-Rauscher (BR) dynamic have been found [1]. Although both are insoluble in BR solution [2], the addition of different masses of PWB linearly decreases the BR oscillation time, while the addition of different masses of PMoB had no effects on the BR reaction. Furthermore, PWB has an identical role as metal catalyst Mn²⁺ in BR reaction and for obtained behavior is probably responsible the different mechanisms of heterogeneous catalysis of these bronzes in oscillatory reaction. Therefore, a deeper investigation was done in order to find the major structural characteristic of these two bronzes by using the XRPD method.

What is so different for these two bronzes, causing dissimilar effects in BR reaction, is it “just” catalytic activity of central cation or there is something more? The XRPD method confirmed very different structures of PWB and PMoB as monoclinic and orthorhombic, respectively [3,4]. This work tries to connect the structural properties of PWB and PMoB with BR oscillatory reaction responses, expanding the usage of oscillatory reaction in material science and catalysis, in general.

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P-25

**DILATOMETRIC STUDY OF NANOSTRUCTURED
Ca_{1-x}Gd_xMnO₃ (X=0.05; 0.1; 0.15; 0.2)**

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Nanocrystalline powders of Ca_{1-x}Gd_xMnO₃ (x=0.05, 0.1, 0.15, and 0.2) have been synthesized by the modified glycine nitrate procedure and pressed into pellets that served as green bodies for a systematic investigation on their structural and microstructural properties [1]. Dilatometric measurements were performed in order to confirm the optimal sintering temperature. Dilatometric curves, besides sintering, are recording superimposed phase transition and linear expansion. Using a dilatometric curve, three temperatures were determined at which the examined sample shows significant changes. At 1055 °C–1194 °C certain second order phase transition is evident, at 1365 °C–1409 °C intensive nitrogen oxide extrusion, and in duration of 86 min at 877 °C heating ramp thorough isothermal holding at 1410 °C until 158 min cooling schedule at 1331 °C sintering is performed. Vickers hardness values were obtained based on the change in the surface area of the diamond pyramid. The results indicate that the hardness of the Ca_{1-x}Gd_xMnO₃ system (x = 0.05; 0.1; 0.15; 0.2) is not conditioned by the amount of doped gadolinium.

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P-26

PALLADIUM DISPERSED IN AMORPHOUS CARBON MATRIX AS THE ELECTROCATALYST FOR HYDROGEN PEROXIDE REDUCTION IN AN ALKALINE MEDIUM

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A method to disperse fine metal particles of Pd in an electrically conductive amorphous C matrix was developed to obtain efficient catalyst for hydrogen peroxide electro-reduction in an alkaline medium. Morpho-structural characterization and chemical composition of composite catalyst, denoted as Pd@AC, were analyzed using SEM, EDX and XRD. The Pd@AC composite was immobilized on the surface of a glassy carbon electrode to examine hydrogen peroxide reduction reaction. The electroreduction of hydrogen peroxide was studied by cyclic voltammetry (CV) and square wave voltammetry in an oxygen-free and air-saturated 0.1 M KOH at a potential range of -0.8 to 0 V. The Pd@AC composite showed pronounced electrocatalytic activity toward the reduction of H₂O₂ in alkaline medium. This study aims to reveal the delicate interaction among diffusion, adsorption phenomena and hydrogen peroxide disproportionation reaction as a heterogeneous process on the contact of three phases: amorphous carbon/palladium particles/electrolyte solution.

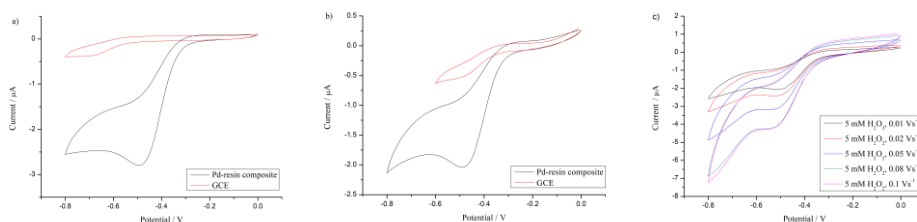


Figure 1. CVs of a Pd@AC GCE (a) in an oxygen-free 0.1 M KOH; (b) 5 mM H₂O₂ in oxygen-free 0.1 M KOH; (c) 5 mM H₂O₂ air-saturated 0.1 M KOH

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P-27

LEAD BASED (PZT) AND LEAD FREE (BZT) COMPOSITES FLEXIBLE FILMS AS LOW-ENERGY PIEZOELECTRIC HARVESTERS

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Various alternative renewable sources such as solar, wind, thermal energy and mechanical vibrations are available for the energy generations. For the last decades, energy harvesters based on piezoelectricity from mechanical vibration are explored extensively for its functionality in energy technologies [1,2]. Flexible piezoelectric energy harvesters (FPEHs) and energy storage system were fabricated by employing solid state synthesized lead-free BZT ($\text{BaZr}_{0.2}\text{Ti}_{0.8}\text{O}_3$) and PZT ($\text{PbZr}_{0.52}\text{Ti}_{0.48}\text{O}_3$) nanopowders prepared by autocombustion method with polyvinylidene fluoride (PVDF) in different volume percentage ($x\text{BZT/PZT}-(1-x)\text{PVDF}$, $x=30, 40, 50$). Both flexible films with quite homogeneous distribution of piezo-active filler were confirmed by XRD and SEM analysis. In addition, the remnant polarization (P_r) and dielectric constant are also investigated to evaluate the breakdown strength in flexible films. The improved dielectric loss tangent (< 0.02) and dielectric permittivity of 120 at room temperature and frequency 1 MHz of BZT-PVDF (50-50) in comparison with neat PVDF films is found beneficial for both energy harvesting and storage. Calculations of storage energies obtained for the investigated materials revealed an increasing trend with increasing amount of active phase (BZT and PZT). The maximum storage energy of 0.11 J/cm^3 and 0.13 J/cm^3 , and energy efficiency (η) of 72% and 39% was obtained for BZT-PVDF (50-50) and PZT-PVDF (40-60) films, respectively. Test of the force impact showing similar output voltage of around 4 V for both, BZT and PZT flexible films.

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P-28

MORPHOLOGICAL AND DIELECTRIC PROPERTIES OF MODIFIED BARIUM TITANATE

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Perovskite ceramics are thoroughly studied and widely used materials in electronic devices. Among them, BaTiO₃ (BTO) is the most commonly employed, due to the high relative permittivity value and DC bias stability. Development of nanostructured materials opened the door for various nano-BTO modifications, with the aim of producing stable material with better dielectric properties. In this research, BTO nanoparticles were chemically functionalized with yttrium-based metal organic salt under different temperature and atmosphere conditions. Scanning transmission electron microscopy with energy dispersive X-ray (STEM-EDX) and conventional transmission electron microscopy (TEM) analyses were used to investigate distribution of yttrium after sintering, and it has been established that core-shell structure has formed after the sintering at 1350 °C. Dielectric properties measurements revealed that samples with higher relative permittivity showed increased DC bias sensitivity. These findings are very useful for further investigation of BTO modification that is necessary for micro- and nano-electronic devices.

P-29

EFFECT OF Ag DOPING ON THE MORPHOLOGICAL AND MAGNETIC PROPERTIES OF CuO NANOSTRUCTURES

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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 using 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 of any re-heating of the sample. A fitting refinement procedure using the Rietveld method was performed which showed the incorporation of Ag^{3+} ions in the CuO crystal lattice, where they substitute 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 CuO with Ag in order to improve further its multiferroic properties. In $\text{Cu}_{1-x}\text{Ag}_x\text{O}$ small changes of magnetic properties were observed if compared to CuO. Transmission electron microscopy (TEM) and the scanning electron microscopy (SEM) were used to determine the particle size and morphology.

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P-30

MAGNETIC PROPERTIES OF Fe₂TiO₅

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Iron(III) titanates are composed of earth-abundant elements and are attracting rapidly growing interest as highly promising candidates for solar-energy as well as optoelectronics applications. Fe₂TiO₅ is generally recognized as potential thermoelectric material. We studied the magnetic properties of pseudobrookite material Fe₂TiO₅ by means of Vibrating Sample Magnetometer and Superconducting Quantum Interferometer Device Magnetometer. The material was synthesized by the sol-gel method and characterized by powder x-ray diffraction. The diffractogram was refined with the help of Rietveld refinement on FullProf Suite. Temperature-dependent ZFC and FC magnetization was measured on SQUID for lower temperature down to 2 K and on VSM for higher temperatures up to 1000 K. A transition was observed at 815 K with a separation between the ZFC and FC curves. Parallely the bifurcation in the isothermal hysteresis measurements indicates that the system exhibits dominant canted AFM (or weak FM) with a small amount of spin glass. The small value of the moment was also pointing towards the canted AFM ordering. Transmission electron microscopy (TEM) and the scanning electron microscopy (SEM) were used to determine the particle size and morphology.

P-31

THE INFLUENCE OF TI-DOPING ON STRUCTURAL AND MULTIFERROIC PROPERTIES OF YTTRIUM MANGANITE CERAMICS

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Hexagonal ($P6_3cm$) yttrium manganite, $YMnO_3$, is a multiferroic material with ferroelectric transition at $T_C \approx 900$ K and antiferromagnetic transition at $T_N \approx 70$ K [1]. Multiferroic behavior attracts a lot of attention because of its potential for various applications [2]. The application possibilities are limited by large microcracking and microporosity of $YMnO_3$ ceramics [3].

In this work, the influence of Ti-doping on structural, ferroelectric and magnetic properties of $YMnO_3$ ceramics was investigated. $YMn_{1-x}Ti_xO_{3+\delta}$ ($x = 0, 0.04, 0.08, 0.10, 0.15, 0.20$) powders were prepared using sol-gel, polymerization complex method from citrate precursors, which were then calcinated at 900 °C for 4 h. The ceramic samples were obtained after sintering for 2 h at: 1400 °C for $YMnO_3$, $YMn_{0.96}Ti_{0.04}O_{3+\delta}$, $YMn_{0.92}Ti_{0.08}O_{3+\delta}$ and $YMn_{0.90}Ti_{0.10}O_{3+\delta}$; 1450 °C for $YMn_{0.85}Ti_{0.15}O_{3+\delta}$; 1470 °C for $YMn_{0.80}Ti_{0.20}O_{3+\delta}$. X-ray diffraction (XRD), transmission and scanning electron microscopy (TEM and SEM) were used for structural and microstructural analysis of samples. Ferroelectric measurements of P(E) loops and leakage currents, and magnetic measurements of zero field cooled (ZFC) and field cooled (FC) $M(T)$ curves, as well as $M(H)$ curves, were enabled multiferroic characterization of ceramic samples.

The samples $x = 0$ and 0.04 are crystallized in a single phased hexagonal structure, ($P6_3cm$), the samples $x = 0.08$ and 0.10 exhibited the presence of both hexagonal phase and rhombohedral phase ($R3c$), and the samples $x = 0.15$ and 0.20 are crystallized in rhombohedral $1 \times 1 \times 3$ superstructure. Ti-doped $YMnO_3$ ceramic samples showed reduced density of microcracks, and inter- and intragranular pores, and large increase in relative density (greater than 90 %) for $YMn_{1-x}Ti_xO_{3+\delta}$ ($x = 0.10, 0.15$ and 0.20) samples. Leakage currents for most of doped samples were lower than leakage current of undoped sample, but the ferroelectric response was not significantly improved. Doping of $YMnO_3$ with nonmagnetic Ti^{4+} led to suppression of antiferromagnetic ordering visible through decrease of the Néel temperature and Weiss parameter and the appearance of weak ferromagnetism.

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P-32

THE DEFECT STRUCTURE AND ELECTRICAL PROPERTIES OF THE SPARK PLASMA SINTERED ANTIMONY-DOPED BARIUM STANNATE

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Barium stannate, BaSnO₃ (BSO), is a perovskite-type alkaline earth metal stannate with almost ideal cubic structure. Appropriate doping can alter this wide band gap material's electrical characteristics and change it either into a proton conductor or n-type semiconductor. In the case of Sb doping on Sn site, BSO becomes n-type semiconductor with high electrical conductivity at 25 °C.

The major drawback of BSO-based ceramics is its low density. The conventional solid state procedure requires long thermal treatments with several intermittent grinding and heating steps at temperatures up to 1600 °C [1].

To overcome this problem, we used Spark Plasma Sintering technique (SPS) for the preparation of BaSn_{1-x}Sb_xO₃, ($x = 0.00$ (BSSO0) and 0.08 (BSSO8)) ceramic samples. The samples structural properties were investigated using XRD (X-Ray Powder Diffraction), XPS (X-Ray Photoelectron Spectrophotometry) and SIMS (Secondary Ion Mass Spectrometry) analyses. XPS analysis revealed the existence of many structural defects, including mixed oxidation states of tin (Sn²⁺/Sn⁴⁺) and oxygen vacancies (V_O) in both BSSO samples.

The electrical properties of the BSSO ceramic samples were investigated in the temperature range of 4–300 K. The presence of oxygen vacancies in the BSSO0 sample led to the absence of the standard activated semiconductor behavior, showing almost linear temperature-dependent resistivity in the examined temperature range. On the other hand, the BSSO8 sample showed almost

temperature-independent resistivity in the range of 70–300 K. This could be a consequence of the presence of many structural defects such as mixed oxidation states of $\text{Sn}^{2+}/\text{Sn}^{4+}$, probably $\text{Sb}^{3+}/\text{Sb}^{5+}$ and significant amount of O^- species, as well as the presence of the low angle grain boundaries found in this sample. The BSSO8 ceramic sample could satisfy the huge demand for the linear resistors with moderate and high conductivity, due to its low and almost constant electrical resistivity in the wide temperature.

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P-33

THE COMPARISON OF ELECTROCHEMICAL PROPERTIES OF ZnMn_2O_4 AND $\text{ZnCr}_{0.15}\text{Mn}_{1.85}\text{O}_4$ IN AN AQUEOUS SOLUTION OF ZnCl_2

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As commercial Li-ion batteries are chiefly composed of a toxic and flammable electrolyte, as well as that Li itself is also toxic and not economical for widespread use due to its rare metal nature, the aim of this work is to create an aqueous Zn-ion battery that contains the same cathode material as used in Li-ion batteries. The materials ZnMn_2O_4 and $\text{ZnCr}_{0.15}\text{Mn}_{1.85}\text{O}_4$ were synthesized through glycine nitrate combustion. The initial material ZnMn_2O_4 was doped with Cr^{3+} in order to diminish Jan-Teller distortion which prevents of Zn^{2+} ions to fully intercalate into their original sites of crystal lattice. The materials were characterized by X-ray powder diffraction (XRPD) and scanning electron microscopy (SEM), while the electrochemical properties were examined through cyclic voltammetry in aqueous solutions of ZnCl_2 . The capacities obtained for the cyclic voltammograms recorded at 10 mVs^{-1} and 50 mVs^{-1} showed that cathode capacities for ZnMn_2O_4 amounted to be 12.4 mAhg^{-1} for 10 mVs^{-1} , as well as 4.8 mAhg^{-1} for 50 mVs^{-1} . The $\text{ZnCr}_{0.15}\text{Mn}_{1.85}\text{O}_4$ demonstrated 45.3 mAhg^{-1} for 10 mVs^{-1} , as well as 12.6 mAhg^{-1} for 50 mVs^{-1} . The results obtained for the capacities of the original and doped material indicate that doping with Cr^{2+} partly diminishes the Jan Teller effect and facilitates the intercalation of Zn^{2+} ions.

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THE IMPROVEMENT OF FERROELECTRIC PROPERTIES OF BiFeO₃ CERAMICS BY DOPING WITH La³⁺ AND Eu³⁺

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Bismuth ferrite is a unique multiferroic material that has a ferroelectric and antiferromagnetic order at room temperature. The rhombohedrally (*R3c*) distorted BiFeO₃ perovskite structure is a result of relative cation displacement along [111] axis of the cubic perovskite structure and relative rotation of two oxygen octahedra in opposite directions around [111] axis [1]. The partial substitution of Bi³⁺ with rare-earth ions can affect the magnitude of lattice distortion and thus the value of electric polarization. The presence of undesirable secondary phases (Bi₂Fe₄O₉ and Bi₂₅FeO₃₉) and structural point defects (oxygen and bismuth vacancies) in pure BiFeO₃ lead to a high leakage current, which deteriorates its ferroelectric properties. Doping with rare-earth elements with large ionic radii is found to reduce the number of the structural defects and thus improve ferroelectric properties [2].

The influence of partial substitution of Bi³⁺ with La³⁺ and/or Eu³⁺ on ferroelectric properties of BiFeO₃ ceramics was investigated. The Bi_(1-x;1-y)La_xEu_yFeO₃ ($x = 0, 0.025, 0.05, 0.10$; $y = 0, 0.025, 0.05, 0.10$) powders were synthesized by hydro-evaporation method, uniaxially pressed at 9 t/cm² and sintered at 835 °C for 3 h. All the ceramic samples showed a rhombohedral structure, without presence of the secondary phases. Their morphology indicated the complete sintering under the given conditions. The grain size and grain shapes differed more depending on the dopant type and amount. The introduction of La³⁺ and/or Eu³⁺ at the site of Bi³⁺ led to such distortions within the rhombohedral lattice that resulted in much greater remnant electric polarization (P_r) in comparison with the undoped sample. The Bi_(1-x;1-y)La_xEu_yFeO₃ ceramic samples with $x+y=0.10$ showed approximately quadratic polarization vs. electric field $P(E)$ hysteresis curves as well as significantly high values of pure ferroelectric polarization P_r , in large electric fields (100–140) kV/cm. The leakage currents of La³⁺/Eu³⁺-doped samples are mostly reduced, especially those doped only with Eu³⁺.

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P-35

ENERGY LANDSCAPE OF THE NOVEL Cr₂SiN₄ COMPOUND DERIVED USING COMBINATION OF THEORETICAL METHODS

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Transition metal nitrides are widely used as hard coatings and CrN is one with many desired properties. Several studies have suggested that the implementation of Si in CrN can significantly improve its performance as a protective coating. According to earlier research, CrSiN coating is comprised of two phases, where the nanocrystalline CrN is embedded in the Si₃N₄ amorphous matrix, but all studies have shown CrSiN only in thin films. Within this study, the bulk Cr-Si-N has been investigated in order to find possible phases of composition Cr₂SiN₄ [1]. Exploration of feasible modification within this system has been performed via global explorations of the energy landscape [2,3] combined with data mining [4] and the Primitive Cell approach for Atom Exchange (PCE) method [5]. Global optimization yielded six energetically favorable candidates ranging from α - to λ -Cr₂SiN₄ phase, where the α -Cr₂SiN₄ type is the lowest in calculated total energy. Data mining based searches led to four structure candidates selected as the most relevant ones, with Al₂MnO₄-spinel-type representing the global minimum in Cr₂SiN₄. Additionally, the Primitive Cell approach for Atom Exchange (PCE) method was employed and three more promising structure candidates have been found within this system. The lowest energy minimum was denoted as the γ -Cr₂SiN₄-type modification but is structurally completely different from the starting γ -phase in the Si₃N₄ system. Since there exists no experimental data that one could compare the results with, the local optimizations were performed on the DFT level employing both, the LDA-PZ and the GGA-PBE functional for comparison. There was good agreement between the results from the two chosen functionals regarding the total energy ranking, space group symmetry, and other structural data. Hence, further investigation of this ternary system is of crucial importance in order to determine the properties of these newly discovered phases and possibilities for industrial and technological applications.

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P-36

TEORETICAL INVESTIGATION OF Y_2O_2S

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In this study, we performed crystal structure prediction and investigate energy landscape of yttrium oxisulfide (Y_2O_2S). Yttrium oxide is one of the most important compounds of yttrium and is widely used in many ceramic materials. An important material Y_2O_2S has been widely used as practical cathode ray tubes since Royce and Smith and Trond et al. [1,2]. In order to predict new crystal structures, global optimizations on the energy landscape of Y_2O_2S have been performed using empirical potentials. Afterwards, a local optimization has been performed using *ab initio* calculations [3]. In particular, various quantum mechanical methods have been applied: Density Functional Theory (DFT) with Local-Density Approximations (LDA) and Generalized Gradient Approximation (GGA), and hybrid B3LYP (Becke, three-parameter, Lee-Yang-Parr) functional. Our calculations were in a good agreement with the experimentally observed trigonal structure ($P-3m1$, no. 164). Furthermore, novel modifications of pure yttrium oxisulfide have been discovered with the change of pressure and/or temperature.

Important feature of yttrium oxisulfide is that those materials are wide-gap semiconductors. Then we need to compute DOS (Density of States) as we discuss the importance of band gaps. Also we included the calculation of the DOS and discuss the band gaps [4].

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P-37

STRUCTURAL AND MECHANICAL PROPERTIES OF HIGH-ENTROPY ALLOYS (HEAS) - ULTRA-HIGH TEMPERATURE CERAMICS (UHTC) ON DFT LEVEL

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High-Entropy Alloys (HEAs) have attracted considerable interest due to the combination of useful properties and enhanced applications, and a few HEAs have already been shown to possess exceptional properties under extreme conditions (e.g. Ultra-High Temperature Ceramic (UHTC)). However, predicting the formation, structures, and stability of HEAs is one of the major goals of recent studies, which is expected to bring discovery of new systems with enhanced properties of the material, with special attention on high temperature and mechanical load. Here, we show an example of high-entropy rare-earth (RE) zirconates with a pyrochlore structure that was examined theoretically and experimentally observed. Theoretical methods were applied to investigate the variable composition of the ordered and disordered pyrochlore structures using quantum mechanics, group action theory, PCAE, and supercell methods. The investigated RE₂Zr₂O₇ compound was successfully fabricated by pressureless and spark plasma sintering. with nominal composition (La_{0.2}Y_{0.2}Gd_{0.2}Nd_{0.2}Sm_{0.2})Zr₂O₇, prepared by simple glycine nitrate procedure (GNP) and characterized using various experimental methods (XRD, SEM, TEM, Raman, etc.). [1] Pyrochlore structures were generated using the Primitive Cell Approach for Atom Exchange (PCAE) method [2] or the supercell approach using the Crystal17 program package [3], and investigation of disordered systems and solid solutions was conducted using the group action theory [4]. Structural optimization on the *ab initio* level was performed using the Crystal17 code, based on a Linear Combination of Atomic Orbitals (LCAO). Density

functional theory (DFT) calculations were utilized in the present study, using the local density approximation (LDA) with Perdew-Zunger (PZ) correlation functional.

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PREDICTION OF STRUCTURE CANDIDATES FOR SiB₆ COMPOUND USING A COMBINATION OF DATA MINING AND THE PCAE METHOD

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Silicon borides represent very appealing industrial materials for research due to their extraordinary features. Discovered at the beginning of the XX century, SiB₆ is considered as one of the most elusive refractory compounds as its crystal structure is yet not fully understood. The first reports suggested a cubic SiB₆, which was followed by an experimentally observed orthorhombic phase, but later studies determined a cubic SiB₆ as an unstable phase and suggested an additional monoclinic *P21/m* space group. In order to predict possible phases within this system of interest, we have undertaken calculations using the ab initio minimization data mining approach [1,2] combined with the PCAE method [3]. Several promising structure candidates have been found and each of the newly found structure candidates was locally optimized on the DFT level, employing the

LDA-PZ and the GGA-PBE functional [4]. Two novel structures have been discovered and are denoted as α -SiB₆-type, appearing in the hexagonal space group *R-3mH* (no. 166), and as δ -SiB₆-type that crystallizes in the space group *P3m1* (no. 156). For these newly discovered phases, there are no previous experimental or theoretical data, but the results of structural relaxation agree between two levels of calculation (GGA-PBE and LDA-PZ). Calculations performed on the experimentally known cubic γ -SiB₆ and recently proposed orthorhombic β -SiB₆ phase are in very good agreement with previous findings. Several earlier studies of this interesting compound suggested its great potential as a high-temperature material and ability to operate in extreme environments. Hence, considering their exceptional properties it is of crucial importance to further investigate this system in order to find new possibilities for future industrial and technological applications.

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P-39

**THEORETICAL STUDY ON ANION SUBSTITUTION OF $\text{TiO}_{1-x}\text{S}_x$
($x = 0, 0.25, 0.5, 0.75$ AND 1) COMPOUNDS AND THE
INFLUENCE OF SULFUR ON CRYSTAL STRUCTURES, PHASE
TRANSITIONS AND ELECTRONIC PROPERTIES**

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Several recent studies of $\text{TiO}_2/\text{TiS}_2$ nanostructures have been reported showing improved properties with applications from electronics and catalysis to solar cells and medicine, while there is a limited number of studies on the crystal structures of $\text{TiO}_2/\text{TiS}_2$ compounds with corresponding properties. Since metal or nonmetal doping of TiO_2 enables the narrowing of the band gap and the TiS_2 has applications as a material for the cathode in rechargeable batteries, hydrogen storage applications and thermoelectric materials, it was interesting to follow the effect of mixing these two end members (TiO_2 and TiS_2) of the $\text{TiO}_{1-x}\text{S}_x$ solid solution and their structures and electronic properties. In order to investigate $\text{TiO}_2/\text{TiS}_2$ mixed compounds as a function of sulfur doping, *ab initio* modelling using DFT method has been performed. In particular, solid solutions of $\text{TiO}_{1-x}\text{S}_x$ ($x = 0, 0.25, 0.5, 0.75$ and 1) with anatase, rutile, and CdI_2 crystal structures were investigated using LDA-PZ and GGA-PBE functionals using the CRYSTAL 17 software package. To create mixed $\text{TiO}_2/\text{TiS}_2$ crystal structures we have used two methods: the PCAE (The Primitive Cell approach for Atom Exchange) method and the supercell approach [1]. Novel phase transitions and predicted structures are presented, and apart from several interesting metastable structures, a very interesting pressure-induced phase transition is found in the TiOS compound [2]. The first description of the electronic properties of the mixed $\text{TiO}_{1-x}\text{S}_x$ compounds in crystal form has been presented and studied through the dependence of semiconducting properties on dopant concentration which will possibly have numerous industrial and technological applications.

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P-40

ENERGY LANDSCAPE EXPLORATION OF NOVEL TERNARY RARE-EARTH COMPOUND LAIO

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Rare earth metals and their compounds and alloys have important applications in various mature markets as well as in high technology markets, so identifying new rare earth compounds and modifications is an important enterprise. Traditionally, this is done experimentally, by synthesizing many new materials in an exploratory fashion and studying their properties. However, this approach is increasingly complemented by theoretical calculations that predict new compounds or modifications without recourse to experimental input [1,2].

The major task here is the general, unbiased prediction of stable crystalline compounds of a chemical system: at which composition does a system form a kinetically and/or thermodynamically stable compound, what are the structural and chemical/physical properties, to what degree is the compound stable, and what will happen if a (metastable) compound undergoes a phase transition? To answer these questions for our system, we investigated its energy landscape, i.e. the (potential) energy as a function of atomic positions in the system.

Crystal structure candidates of LaIO are found using the global optimization (GO) method - simulated annealing [3] using empirical potentials as implemented in the G42+ code [4] is chosen. Relevant candidates identified by GO, threshold runs or data mining are locally optimized on the *ab initio* level (CRYSTAL17 package [5] was used for DFT calculations with various exchange-correlation functionals). Such explorations were successfully performed in the past using empirical and *ab initio* potentials [6,7]. For the most promising candidates, *ab initio* calculations of their properties were performed, such as the equation of state ($E(V)$ curves), band gaps, band structures, etc.

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P-41

SINTERING OF TUNGSTEN BASED REFRACTORY COMPOSITE

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In this work, WSi_2 and W_5Si_3 are used as additives for the sintering of WC powders. Tungsten silicides were made from powders, following a simple synthesis procedure. Optimal synthesis conditions – the heating temperature and duration of heating - were found through a series of experiments. The synthesized tungsten silicides were added to the commercial WC powder in different weight ratios - 5 and 10 wt.% of the silicide mixture. The powder mixtures were spark plasma sintered at 1600 °C, at a heating rate of 100 °/min under a load of 50 MPa, 5 minutes in vacuum. Scanning electron microscopy of sintered samples showed that porous structures were obtained, but they exhibit a great cavitation erosion resistance. X-ray diffractometry of polycrystalline sintered samples showed that W_5Si_3 originally present as an additive converted to WSi_2 . The resistance of sintered materials due to cavitation erosion was tested, and it was shown that the obtained samples are extremely resistant to these damages, which was confirmed not only by measuring the change in mass but also by profilometric analysis, monitoring roughness parameters, and analysis of the obtained 3D surface image. Nanoindentation measurements enabled the calculation of Young's modulus of elasticity as well as the hardness of the sintered materials.

P-42

PHASE TRANSFORMATIONS DURING CYCLIC ANNEALING OF Ti₃Al-BASED INTERMETALLIC

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Alterations that emerged in the intermetallic Ti₃Al-based alloy microstructure during the cyclic annealing at 600 °C and 900 °C in the air atmosphere were studied by combining experimental and theoretical methods. The phase transformations in the Ti-24Al-11Nb (at.%) alloy microstructure were monitored during the alloy high-temperature processing up to 120 h. The conducted cyclic annealing resulted in the external oxide scale formation and the microstructural features alteration. Obtained experimental results indicated that the annealing temperature and duration significantly affected the external scale composition and structure, as well as the alloy phase composition. Namely, the alloy microstructural characterization revealed that a starting two-phase $\alpha_2+\beta$ microstructure changed to a great extent during the cyclic annealing. The increase of the cyclic annealing temperature induced the intensive $\alpha_2\rightarrow\beta$ phase transformation and as a result, new α_2'' and O-Ti₂AlNb phases appeared in the investigated alloy microstructure. The experimentally observed appearance of the O-Ti₂AlNb phase in the Ti₃Al-based alloy microstructure was confirmed by the results of theoretical investigations. *Ab initio* modeling also enabled the prediction and study of the additional structures in the O-Ti₂AlNb compound using the first-principles calculations.

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**EFFECT OF Cu DOPING ON MICROSTRUCTURAL,
THERMOELECTRIC AND MECHANICAL PROPERTIES
OF NaCo₂O₄ CERAMICS**

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Ceramic samples of NaCo_{2-x}Cu_xO₄ (x = 0, 0.01, 0.03, 0.05) were obtained after calcination of powder precursors synthesized by a mechanochemically assisted solid-state reaction method (MASSR) and a citric acid complex method (CAC). Effects of small concentrations of Cu doping and the above-mentioned syntheses procedures on the microstructural, thermoelectric and mechanical properties were observed. The electrical resistivity (ρ), the thermal conductivity (κ) and the Seebeck coefficient (S) were measured simultaneously in the temperature gradient (ΔT) between hot and cold side of the sample, and the figure of merit (ZT) was subsequently calculated. ZT of the CAC samples was higher compared with the MASSR samples. The highest ZT value of 0.061 at $\Delta T = 473$ K was obtained for the sample with 5 mol% of Cu prepared by the CAC method, and it was 1.7 times higher than the highest value obtained for the MASSR sample with 3 mol% of Cu ($ZT = 0.036$ at $\Delta T = 473$ K). The CAC samples showed better mechanical properties compared to the MASSR samples due to the higher hardness of the CAC samples which is a consequence of homogeneous microstructure and higher density obtained after sintering of these samples. The results confirmed that, besides the concentration of Cu, the synthesis procedure considerably affected the microstructural, thermoelectric and mechanical properties of NaCo₂O₄ ceramics.

P-44

THERMAL PROPERTIES OF Ag DOPPED GLASS-CERAMIC MATERIAL FROM As-Te-Se SYSTEM

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Thermal characterization of glass ceramic material $\text{As}_{40}\text{Te}_{30}\text{Se}_{30}$ doped with 1 at.% of silver in temperature range from 300 K to 650 K was done. This glass was selected and synthesized as potentially new material that could be used for phase-changing memories and for photovoltaic cells in solar panels. In order to assess the possibility of application, the determination of thermal parameters in this composition is imposed as an imperative. The DSC measurements performed with different heating rates, revealed three thermally induced processes: glass transition, crystallization of the structural units and melting of formed crystalline phases. The glass transition process, which is detected in DSC images as a weakly pronounced endothermic effect, was characterized with onset glass transition temperature, T_g and apparent activation energy, E_g . Apparent activation energy of complex crystallization process, E_c , was determined according to models proposed by Kissinger [1] and Mahadevan [2]. Value of E_c was 113(3) kJ mol⁻¹. Also E_c was analysed using isoconersional (model free) method [3, 4] which pointed to the complex nature of the crystallization process. Characteristic temperatures served as the basis for the calculation of the thermal stability parameters of the glass towards crystallization. Thermal stability was estimated according to the parameter proposed by Dietzel, ΔT parameter [5]. Value of this parameter was 100.9(7) K at heating rate of 20 K min⁻¹. A comparison with glass without silver ($\Delta T = 86.5(7)$ K) showed that the introduction of silver leads to an increase of the thermal stability.

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P-45

EFFECT OF TWO ACTIVATION METHODS ON MECHANICAL PROPERTIES OF HIGH VOLUME FLY ASH BINDERS

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In this work, the effects of mechanical and chemical activation, as well as their combination, on the mechanical properties of high volume fly ash (HVFA) binders were investigated. Mechanical activation was conducted by grinding fly ash (FA) in a planetary ball mill. It resulted in drastic particle size reduction and increase in specific surface area of the FA. Morphology of FA particles, examined by scanning electron microscope, was also changed. The chemical activation was carried out by adding sodium sulfate to the dry mass of the binder. Effects of the activation methods on mechanical properties of the resulting binders were examined by determining setting time and compressive strength of HVFA mortars. The results showed that both activation methods lead to significant decrease in setting time and increase in early compressive strength, especially when combination of both of the activation methods was applied. Thus, properties of HVFA binders that have been limiting their use in the construction industry, i.e. long setting time and low early strength, were improved by using mechanical and chemical activation.

P-46

SYNTHESIS OF GEOPOLYMERS BASED ON SPENT CATALYST FROM PETROL REFINERIES

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Geopolymers are class of alkali activated materials obtained by alkali activation of aluminosilicate precursors. The main product of alkali activation reaction is amorphous aluminosilicate, “geopolymer” gel. Due to highly interconnected, three-dimensional structure of aluminosilicate gel, geopolymers can show high compressive strength and good durability, and can be regarded as alternative to Portland cement in some applications.

Spent catalyst from fluid catalytic cracking process (spent FCCC) is an inorganic by-product from petrol refineries. It consists mostly of zeolite (usually faujasite) and amorphous aluminosilicate matrix, and SiO₂ and Al₂O₃ make about 90 % of its chemical composition.

In this work, spent FCCC was used as a precursor for geopolymer synthesis. Prior to chemical activation, spent FCCC was ground in a planetary ball mill. Alkali activation was carried out using sodium silicate solutions with different SiO₂/Na₂O ratios. The reaction was performed at 65 °C for 24 h. Synthesized geopolymer paste samples were analyzed using scanning electron microscopy and X-ray powder diffraction. The results showed that alkali activation of the spent FCCC sample converted zeolitic phase to aluminosilicate geopolymer gel. Determination of the mechanical properties of the synthesized geopolymer mortar samples indicated that using the optimal modulus of the activating solution can produce geopolymers with compressive strength higher than 70 MPa. The obtained results confirmed potential to use spent FCCC as starting material for geopolymer production.

P-47

DETERMINING THE ABSOLUTE AGE AND TYPE OF MAGMA OF TRIASSIC ANDESITES OF ČADINJE USING U/Pb DATING AND BACKSCATTER METHODS ON ZIRCON SAMPLES

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Zircon ($ZrSiO_4$) is a mineral with a variety of applications in a wide range of industries but is rare as a natural mineral thus to fulfill the demand for this rare material mostly synthetic zircon is used. The aim of this work is to study the microstructure of natural zircon found in andesites from Čadinje, Prijepolje to determine the absolute age, the type of magma that the zircon was formed in and a possibility of using it as a natural precursor in zircon based ceramics.

For the purposes of this work, the method used for determining the absolute age of porphyrites (andesites) is U/Pb dating method used on zircon samples which are extracted from the andesites. The morphology of the zircon crystals was analyzed using backscatter method (SEM) for determining the classification and internal structure of zircons as well as the type of magma in which the crystallization took place using the typology method. Optical test using a polarizing microscope was used to determine wall-rock alterations which were multiphase and very complex.

These analyses are very important as they help for better understanding of distribution / zonation of zircons and alteration minerals in similar magmatic rocks, but also ore minerals, because it can indicate the temperatures of ore-bearing solutions, and thus the time of sulfide deposition of certain elements.

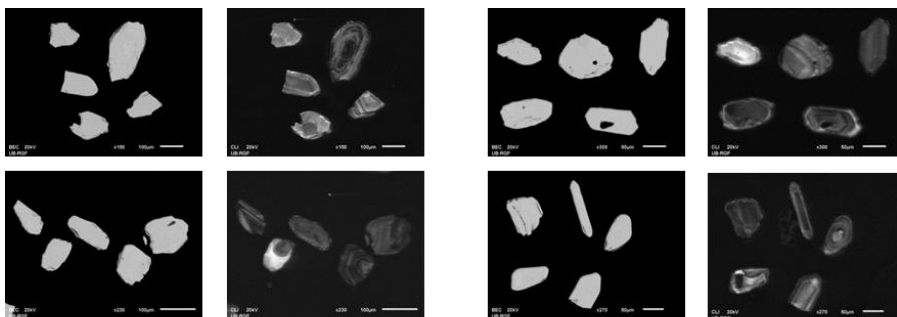


Figure 1. SEM micrographs of zircon from andesites of Čadinje

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