# CMSE 2021

The 10th Global Conference on Materials Science and Engineering

# CONFERENCE PROGRAM

## ONLINE - Microsoft Teams Meeting

**August 1-4, 2021**

**Eastern European Summer Time (EEST)**

***For CMSE2021 Academic Exchange Only**

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|---|---|
| 08:30-08:35 | **Opening & Welcome Speech**<br>***General Chair:***<br>***Prof. Sigitas Tamulevičius,*** *Member of the European Materials Research Society. Professor of the Physics Department, Kaunas University of Technology (KTU), Republic of Lithuania* |
| 08:35-09:15 | **Keynote Speech 1:** Intelligent Materials & Systems: Healthcare<br>***Prof. Seeram Ramakrishna,*** *FREng, FBSE, Everest Chair, Circular Economy Taskforce, National University of Singapore, Singapore* |
| 09:15-09:55 | **Keynote Speech 2:** Efficient Color-tunable Emission from Rare Earth Doped Gallium Oxide Films<br>***Prof. Qixin Guo****, Department of Electrical and Electronic Engineering, Director of Synchrotron Light Application Center, Saga University, Japan* |
| 09:55-10:35 | **Keynote Speech 3:** High Entropy Alloys Obtained by Powder Metallurgy<br>***Prof. José M. Torralba****, Department of Materials Science and Engineering, The Universidad Carlos III de Madrid (UC3M), Senior Scientist at IMDEA Materials Institute, Spain* |
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| 10:40-13:30 | **Oral Session 1: Materials for Electronics, Optoelectronics, Semiconductors** |
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***MS Teams: http://www.academicconf.com/Identity/Account/Login?confName=cmse2021***

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## August 4, 2021 / Eastern European Summer Time

***MS Teams: http://www.academicconf.com/Identity/Account/Login?confName=cmse2021***

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| 14:15-18:05 | **Oral Session 5B: Nanostructured Materials, Sensors** |

# Part II Keynote Speeches

## Keynote Speech 1: Intelligent Materials & Systems: Healthcare

***Prof. Seeram Ramakrishna***

**FREng, FBSE, Everest Chair, Circular Economy Taskforce, National University of Singapore, Singapore**

**Biography:** Professor Seeram Ramakrishna, FREng, FBSE, Everest Chair is among the top three impactful authors at the National University of Singapore, which is ranked among the top ten engineering universities of the world. He is the Director of Center for Nanotechnology & Sustainability. Listed among the top three scientists of the world in Biomedical Engineering based on career-long impact of researchers or c-score. Thomson Reuters identified him among the World's Most Influential Scientific Minds. His Google Scholar citations reach ~116,000 and H-index 160. Clarivate Analytics recognized him among the Top 1% Highly Cited Researchers in the world in materials science and cross-fields categories. Microsoft Academic ranked him among the top 50 impactful persons out of three million materials researchers worldwide. He co-authored books An Introduction to Biomaterials Science & Engineering; Medical Devices- Standards, Regulations and Practices; Biomaterials- A Nano Approach; and An Introduction to Bio-composites. He is the Biomaterials Editor of Elsevier Current Opinion in Biomedical Engineering. He is regarded as the guru of electrospinning and nanofibers for diverse applications. Prof. Ramakrishna is an elected Fellow of UK Royal Academy of Engineering (FREng); Singapore Academy of Engineering; Indian National Academy of Engineering; and ASEAN Academy of Engineering & Technology. He is also an elected Fellow of American Association of the Advancement of Science (AAAS); ASM International; American Society for Mechanical Engineers (ASME); American Institute for Medical & Biological Engineering (AIMBE); Institution of Mechanical Engineers, IMechE and Institution of Materials, Minerals & Mining, IoM3, UK; ISTE, India; and International Union of Biomaterials Science & Engineering (FBSE).

**Abstract.** Biomaterials development is synonymous with improvements in the healthcare outcomes and well-being of human race on planet earth. This can be appreciated from the critical importance of personal protection equipment (PPE), facemasks, temperature measurement devices, sensors, diagnostic kits, emergency medical care, vaccines, and medicines used worldwide to eradicate the COVID19 pandemic (https://doi.org/10.1016/j.bios.2020.112731). The isolation and social distancing measures due to COVID19 also affected the emotional and mental wellbeing of people and healthcare professionals. A technology start-up company Neuralink (https://www.neuralink.com/) announced a neural interface or in-brain device that could potentially solve neurological challenges from memory loss, hearing loss and vision loss to paralysis, depression and brain tissue damage. Moreover, it is envisaged that with further research and innovation the brain-machine interface will enable humans to control external devices such as computers and phones via thoughts. Aforementioned enabled by the advances in the field of biomaterials science & engineering, and availability of thousands of diverse biomaterials.

History of biomaterials is akin to 300,000 years of existence of human race on the planet earth

(https://doi.org/10.1080/07373937.2020.1829885). For most part, humans relied on easily sourced materials from the immediate nature. Over the recent 2,000 years, humans learnt to process raw materials sourced from the nature into useful metals & alloys and ceramics. More recently, i.e. 20th century, humans learnt to produce a range of synthetic polymers and their composites with ceramic additives. Via trial and error, humans found out that a few of these numerous engineered materials are suitable for treating or augmenting diseased or damaged tissues of the human body. As they are not purposefully designed to appropriately interact with the host tissues of human body, they are denoted as 'passive biomaterials'. In recent three decades, building on the advances in molecular biology, biochemistry, stem cells, biotechnology and biomedical engineering, the biomaterials are purposefully designed to interact with the host tissues and cells in specific ways for realising improved health care outcomes. They are designed by mimicking the microstructure and underpinning functional mechanisms of natural and healthy tissues of the human body. Hence, we can denote them as 'engineered biomimetic biomaterials', which are being experimented in the emerging fields of tissue engineering, regenerative medicine, stem cells, and nanomedicine. Moving forward, 'intelligent biomaterials' are necessary to meet the growing demands of healthcare. Wherein, an intelligent biomaterial or cognitive biomaterial can be described to have the ability to be aware of external stimuli and learn from it to optimize response behaviors for achieving its choices or goals to the greatest extent for optimal performance. Intelligent biomaterials are capable of processing external signals as well as internally generated signals in order to take actions that maximize its chance of successfully achieving its goals (Liu et al., Intelligent Materials, Matter, 2020, https://doi.org/10.1016/j.matt.2020.07.003). Currently, available protein and lipid based bioactive materials, shape memory materials, piezoelectric materials, photoelectric materials, and thermoelectric materials are nascent examples of intelligent biomaterials. Often, the scientific literature refers them as smart biomaterials. Recent advances in quantum biology (https://www.technologyreview.com/2019/11/09/238365/a-natural-biomolecule-has-been-measured-acting-in-a-quantum-wave-for-the-first-time), and examples of intelligent materials in the nature inspire the biomaterials community to advance the domain of intelligent biomaterials.

This lecture will illustrate the intelligent biomaterials & systems necessary to enable futuristic healthcare and well-being. Moreover, the potential for more effective antimicrobial and antiviral surfaces and treatments; regenerative medicine; neural interfaces & neuroprosthetics; next generation medical devices; wearables and personalised healthcare will be deliberated in this lecture.

## Keynote Speech 2: Efficient Color-tunable Emission from Rare Earth Doped Gallium Oxide Films

***Prof. Qixin Guo***
***Department of Electrical and Electronic Engineering, Director of Synchrotron Light Application Center, Saga University, Japan***

**Biography:** Prof. Dr. Guo received B. E., M.E., and Dr. E degrees in electronic engineering from Toyohashi University of Technology in 1990, 1992, and 1996, respectively. He is currently a Professor of Department of Electrical and Electronic Engineering, Saga University as well as Director of Saga University Synchrotron Light Application Center. His research interests include epitaxial growth and characterization of semiconductor materials. Prof. Guo has published more than 300 papers in scientific journals including Nature Communications, Advanced Materials, Physical Review B, and Applied Physics Letters.

**Abstract.** Color-tunable light emitting diodes are of high interest because they would rely on primary color mixing rather than blue-light stimulated phosphors, avoiding impact on human sleeping habits and circadian rhythms caused by excessive blue light, and allowing for smaller pixels in display applications. Color-tunable light emitting diodes can be fabricated by using InGaN with different indium concentration as luminescence layers. However, the emission wavelength is unstable due to its temperature dependence of bandgap.

Rare earth (RE) doped semiconductors, which exhibit strong and sharp emission due to intra-4f-shell transitions in RE ion cores, have potential applications in color display and luminescence devices. Historically, much effort has been made to produce visible color emission using RE doped GaN. It has been reported that the luminescence efficiency of dopant emissions could be highly improved with a wide bandgap host. Moreover, the wide bandgap semiconductors exhibit highly thermal and chemical stability, which make them ideal hosts for Er ions. We have demonstrated that green and red emissions are clearly observed from the Er and Eu doped $Ga_2O_3$ films respectively. We found that the normalized emission intensity of the RE doped $Ga_2O_3$ films has a smaller temperature variation compared to that of the RE doped GaN films. In this talk, we report on the structure, surface morphology and optical properties of these RE doped $Ga_2O_3$ films. Recent progress on the characteristics of the color-tunable light emitting diodes by using the multilayer structured RE doped $Ga_2O_3$ films will also be presented.

## Keynote Speech 3: High Entropy Alloys obtained by Powder Metallurgy

***Prof. José M. Torralba***
***Department of Materials Science and Engineering, The Universidad Carlos III de Madrid (UC3M), Senior Scientist at IMDEA Materials Institute, Spain***

**Biography:** José Manuel Torralba, Professor of Materials Science and Engineering in the Department of Materials Science and Engineering at the Universidad Carlos III de Madrid (UC3M) and Senior Scientist at IMDEA Materials Institute. Prof. Torralba is Fellow in the two most important Powder Metallurgy associations in the world: FAPMI and FEPMA (first European to be Fellow at the same time in Europe and USA). He has participated in more than 80 International Advisory Committees at International Conferences, in about 35 competitive funded projects (among which five EU-projects and one NSF-USA project) and in several research evaluation panels (including the EU Research Framework Programmes) some of which in Israel and New Zealand. Throughout his career, Prof. Torralba has constantly striven for a holistic approach, being involved in a wide number of academic activities: teaching, research, innovation, university management and management of research programmes and science communication. He also regularly participates in activities related to mentoring, research integrity, new ethics in science and to the promotion of healthy conditions in research labs. He has been an active supervisor of PhD students and has created a good international network of former students in academia and industry. Prof. Torralba also collaborates regularly with two NGOs (supporting a secondary school in Kenya and providing scientific divulgation lectures in jails).

**Abstract.** High entropy alloys (HEAs) are a new family of metallic materials that have attracted important attention in the last 16 years. This materials engineering' field has increased enormously, and today, more than 11,000 papers and patents related to this topic have been published; additionally, different subbranches such as "refractory high entropy alloys" and "eutectic high entropy alloys" have emerged. HEAs were first developed via ingot metallurgy, but in this family of alloys, which uses five or more elements and many with dissimilar density, it is difficult to obtain a good level of solubility during melting and to avoid segregation during solidification. In this case, powder metallurgy (PM) is a forming technology that can avoid many problems present in conventional ingot metallurgy, offering a better microstructural control, the possibility of nanocrystalline materials or the capability of developing metal matrix composites without the segregation issue. The first papers related to HEAs manufactured by PM appeared in 2008. PM offers some particular advantages over ingot casting, including two particular benefits over other forming techniques: 1) it can be applied when metals with dissimilar densities must be used, which is the case when lightweight HEAs are developed and 2) it can be applied when many metals with notably high melting points are involved, the so-called refractory HEAs. In this decade, more than 400 papers have been published on high entropy alloys manufactured by PM techniques; more than 60 of these papers report an additive manufacturing approach (not including the use of powders to develop laser cladding coatings).

# Part III Online Oral Presentations

## Online Oral Presentation Guidelines

- Online Oral Presentation will be conducted via Microsoft Teams Meeting (Click to see how to join CMSE 2021 via MS Teams).
- All presenters are requested to reach the Online Session Room prior to the scheduled time and deliver their presentations on time.
- The presentation timetable is shown in **Eastern European Summer Time.**
- If a presenter is not able to show up via MS Teams, the session chair / conference secretary will download and play the pre-recorded video presentation during his/her scheduled presentation time; if listeners have questions about the presentation, please contact the conference secretary to forward the questions.
- If a presenter cannot show up on time or have problems with Internet connection, the session chair has the right to rearrange the presentation order and let the next presenter start.
- Signed and stamped electronic presentation certificate would be issued and delivered via e-mail after presentation.

## Best Oral Presentations Award

The session chair will select one best oral presentation from his/her session based on the following criteria and the "votes" on the conference website:

- ✓ Research Quality
- ✓ Presentation Performance
- ✓ Presentation Language
- ✓ PowerPoint Design

**Best Presenters will receive an official certificate and free registration to the CMSE 2022.**

## Oral Session 1: Materials for Electronics, Optoelectronics, Semiconductors

**Time: 10:40-13:30, August 2, 2021.** Eastern European Summer Time.
**Session Chair: Prof. Yaovi GAGOU, Université de Picardie Jules Verne, France**
***Session Room Link: http://www.academicconf.com/teamslink?confname=cmse2021***

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|---|---|
| 10:40-11:05 **CMSE4465** | Superconducting Correlations of the Edge States in a Topological Insulator<br>*Prof. Victor Kagalovsky, Department of Electrical and Electronics Engineering, Shamoon College of Engineering, Israel* |
| 11:05-11:20 **CMSE4508** | Research on Suppressing Brittle Fracture and Implementing Ductile Mode Cutting for Improving Surface Quality at Silicon Wafers Manufacturing<br>*Dr. Andrii Kovalchenko, Institute for Problems of Materials Science, Ukraine* |
| 11:20-11:45 **CMSE4498** | Controlling the Structure and Optical Properties of Thin Organic Films<br>*Dr. Kostyantyn Grytsenko, Department of Functional Materials and Nanostructures, V.E. Lashkaryov Institute of Semiconductor Physics, Ukraine* |
| 11:45-12:10 **CMSE4609** | Mixed Ferroelectric Oxides for Electrocaloric Cooling Devices<br>*Prof. Yaovi GAGOU, Laboratory of Condensed Matter Physics (LPMC), Université de Picardie Jules Verne, France* |
| 12:10-12:35 **CMSE4481** | The Rise of 2D Indium Selenide: a Novel van der Waals Material for Electronics and Optoelectronics<br>*Dr. Zakhar Kudrynskyi, School of Physics and Astronomy, University of Nottingham, United Kingdom* |
| 12:35-13:00 **CMSE4552** | Influence of Multiferroic and Ferromagnetic Dopants on the Structural and Superconducting Properties of the YBCO Superconductor<br>*Dr. Paweł Pęczkowski, Institute of Physical Sciences, Faculty of Mathematics and Natural Sciences, Cardinal Stefan Wyszyński University, Poland* |
| 13:00-13:15 **CMSE4510** | Electrical and Optical Investigations in Strontium Phosphate Glasses<br>*Dr. Zahra Ramzi, SCiMATOP, Chemistry Department, Faculty of Science, Cadi Ayyad University, Morocco* |
| 13:15-13:30 **CMSE4604** | Dynamic Responses of Electrical, Dielectric and Magnetic Properties of La Substituted Ni-Cu-Cd Bulk Ceramics with Theoretical Justifications<br>*Mr. Faishal Mahmood, Department of Physics, Chittagong University of Engineering and Technology, Bangladesh* |

# Abstracts of Session 1

**CMSE4465**
**Superconducting Correlations of the Edge States in A Topological Insulator**

V. Kagalovsky[1,*] and I. V. Yurkevich[2]
[1]*Department of Electrical and Electronics Engineering, Shamoon College of Engineering, Israel*
[2]*School of Engineering & Applied Science, Aston University, UK*

**Abstract.** We study the stability of multiple conducting edge states in a topological insulator against perturbations allowed by the time-reversal symmetry. A system is modeled as a multi-channel Luttinger liquid, with the number of channels equal to the number of Kramers doublets at the edge. Assuming strong interactions and weak disorder, we first formulate a low-energy effective theory for a clean translation-invariant system and then include the disorder terms allowed by the time-reversal symmetry. In a clean system with $N$ Kramers doublets, $N-1$ edge states are gapped by Josephson couplings and the single remaining gapless mode describes the collective motion of Cooper pairs synchronous across the channels. Disorder perturbation in this regime, allowed by the time-reversal symmetry is a simultaneous backscattering of particles in all $N$ channels. Its relevance depends strongly on the parity if the number of channel $N$ is not very large. Our main result is that disorder becomes irrelevant with the increase of the number of edge modes leading to the stability of the edge states' superconducting regime even for repulsive interactions.

**Keywords:** Topological insulator, Superconducting edge state, Parity.

**CMSE4508 To avoid repeatability issues, this abstract will be available after the full paper is published in the conference proceedings.**

**CMSE4498**
**Controlling the Structure and Optical Properties of Thin Organic Films**

Kostyantyn Grytsenko[1,*], Yurii Kolomsarov[1], Peter Lytvyn[1], Yurii Slominski[2]
[1]*Department of Functional Materials and Nanostructures, V.E. Lashkaryov Institute of Semiconductor Physics, Nauki pr. 41, Kyiv, Ukraine*
[2]*Department of Colour and Structure of Organic Compounds, Institute of Organic Chemistry, Murmanska str. 5, Kyiv, 02660 Ukraine*

**Abstract.** Solar cells, organic light emitting diodes and field effect transistors represent some of applications of organic films in optoelectronic. Deposition in a vacuum have been used for production of inorganic films. Deposition in a vacuum of organic film is necessary for production of hybrid organic-inorganic devices. Thin film from small molecule (dye) can be made by wet and vacuum deposition. Polymer film can be deposited by wet method only with a few exceptions: homopolymers,

including the most stable fluoropolymers (FP). Attaining the properties of precursor to deposited films is extremely important. Structure and morphology of deposit plays crucial role in film properties, so creation of the methods to control the structure of organic films is important task. Thin FP films with surface smoothness at nanoscale were produced by evaporation of FP in vacuum. Varying the deposition conditions and polymers, refractive index, morphology and hardness were varied.

Change of end group in dye molecule and substrate type resulted in different growth kinetics and thermodynamics. Islands, crystals, self-organized nanostructures and dichroic nanowires were obtained (Figure).

Report discusses purposeful control of organic deposits morphology and optical properties.

**Keywords:** Deposition in vacuum, Thin film, Dye, Polymer, Morphology.

**CMSE4609**
**Mixed Ferroelectric Oxides for Electrocaloric Cooling Devices**

Yaovi GAGOU
*Laboratory of Condensed Matter Physics (LPMC), Université de Picardie Jules Verne, France*

**Abstract.** Cooling systems involve heat transfer gases describing a classic Carnot cycle. These gases are unfortunately harmful and cause the "greenhouse effect" as soon as they escape from their containers during production or in the various heat exchange devices already manufactured. It is therefore urgent to find alternatives; less energy consuming and environmentally friendly solutions.
Ferroelectric materials constitute a solution due to their electrocaloric property in solid phase, described by the presence of permanent dipolar moments. The ferroelectric-paraelectric phase transition takes place by a crystal symmetry break and a heat exchange takes place in the material, in a reversible process which can be exploited for cooling applications by control of applied electric field. To the latent heat at phase transition is added the temperature variation due to the entropy change, that compensates the creation of the entropy of phonons in the material, in a reversible transformation with a constant internal energy.

In order to have amplification of the electrocaloric effect, several avenues are currently being explored, in particular, studies on composites, multiferroics and heterostructures.

In this presentation, we will show the recent results obtained on ceramics manufactured from a powder mixture of nanometric grain size ferroelectric oxides well-chosen to have very closed Curie temperature (for example in BCT and BCZT). We will demonstrate the role of hard and soft ferroelectric behaviour on ECE responsivity.

**CMSE4481**

## The Rise of 2D Indium Selenide: a Novel van der Waals Material for Electronics and Optoelectronics

Zakhar Kudrynskyi[1,2,*]
[1]*School of Physics and Astronomy, University of Nottingham, United Kingdom*
[2]*Advanced Materials Research Group, Faculty of Engineering, University of Nottingham, United Kingdom*

**Abstract.** Atomically thin layers of van der Waals crystals and their heterostructures, generally called as two-dimensional (2D) materials, have attracted enormous interest for nearly two decades now. Following the discovery of graphene, the first known truly 2D crystal, there has been a constant search for novel related materials to enrich the library of 2D compounds with new properties. Most attention has been focused on graphene itself, as well as semiconducting crystals of transition metal dichalcogenides and wide-gap insulator hexagonal boron nitride. However, during the recent years an exciting and rapidly growing development in the family of 2D materials involves indium selenide (InSe). This semiconducting crystal has a bandgap energy that increases markedly with decreasing layer thickness, enabling fabrication of devices with high broad-band photoresponsivity. In addition, it has a relatively low mass conduction band electrons and high electron mobility even in atomically thin films, larger than in silicon-based field effect transistors.

This talk reviews my recent research on this new 2D semiconductor. From the fundamental studies of 2D layers and heterostructures to the demonstration of prototype devices, I will discuss how this system can provide a platform for scientific investigations and new routes to ultra-thin electronics and optoelectronics, including high mobility field effect transistors and hybrid multi-layered structures for quantum metrology and photosensing.

**Keywords:** 2D crystals, InSe, van der Waals heterostructures, Quantum effects.

**CMSE4552**

## Influence of Multiferroic and Ferromagnetic Dopants on the Structural and Superconducting Properties of the YBCO Superconductor

Paweł Pęczkowski
*Institute of Physical Sciences, Faculty of Mathematics and Natural Sciences, Cardinal Stefan Wyszyński University, Poland*

**Abstract:** Optimizing high-$T_c$ superconducting materials for the production of controlled nanodevices is critical for industrial applications. In my presentation I will present the results of our group research showing the effect of a small amount of $YMnO_3$ (YMO) multiferroic from 0.1 wt% to 5.0 wt% on the change of microstructural and superconducting properties of the basic high-$T_c$ $YBa_2Cu_3O_{7-\delta}$ (YBCO) superconductor. The Raman spectra measurements showed a slight deterioration of the YBCO–YMO superconducting state in the total YMO content, which is due to the disappearance of the orthorhombic phase seen as the O(4) band shifting towards higher wave numbers. It was found from magnetic measurements that a small addition of YMO (about 1.0 wt%) Does not significantly change the

properties of the superconducting YBCO crystallites, and most composites show a critical temperature ($T_c$) close to 92 K.

The presentation will also discuss the results of the diffusion process between YBCO and Fe particles in the amount of 1.0 wt% to 25.0 wt%. Fe diffusion into YBCO arrays can be fundamental to multilayer systems with YBCO|Fe-stop interfaces. The test results (X-ray diffraction and Mössbauer spectroscopy) showed that the orthorhombic structure of YBCO assumes 3.0 wt%. Fe, while with a higher Fe content, the formation of $BaFeO_{3-\delta}$ and iron oxides was observed. The measurements also confirmed the strong suppression of superconductivity in YBCO-Fe materials containing more than 7 wt% Fe. Thanks to the XAS absorption edge research carried out at the "Solaris UJ" Synchrotron Center in Kraków, the valence of $Cu^{2+}$ was confirmed, and a contribution of the 2*p*3*d*10L final states was evidenced, (where L - stands for ligand hole), which provides crucial information on the mobility of electrical carriers from the Cu–$O_2$ planes.

**Keywords:** High-$T_c$ superconductors, Multiferroic and iron compositions, Ceramics materials, Diffusivity, Structure and magnetic properties, Spectroscopic measurements.

**CMSE4510**
**Electrical and Optical Investigations in Strontium Phosphate Glasses**

Zahra Ramzi
SCiMATOP, *Chemistry Department, Cadi Ayyad University, Faculty of Science Semlalia Marrakech, Prince My Abdellah B.P.2390 Marrakech 40000 Morocco*

**Abstract.** Phosphate glasses have superior properties such as high refractive index, high ultraviolet (UV) transmission, high electrical conductivity, low melting temperature and low glass transition temperature, which make them suitable candidates for technological applications such as optical fibers for data transmission, host glasses for solid state lasers, luminescent solar energy concentrators, immobilization of nuclear wastes, solid state batteries and glass-to-metal sealing. Poor thermal stability against crystallization, low chemical durability, volatile and hygroscopic nature of phosphate glasses limit their extensive practical applications. These properties can be improved by introducing different metal oxides into the glass matrix.

In this work, the strontium phosphate glasses were elaborated by the melt quenching technique. The glasses were characterised by powder X-ray diffractometry. The effects of the substitution of the SrO ions by the $Bi_2O_3$oxide on the wide range of properties of these glasses were investigated. The infrared spectroscopy was performed to identify the different units developed in the amorphous network. Electrical properties have been studied using impedance spectroscopy. Analysis of the UV–VIS data describes the action role of $Bi_2O_3$ as a network modifier in the low concentration range (x= 10 mol%), while it starts to act as a network former in the higher concentration range.

**Keywords:** Phosphate glasses, Optical, Dielctric.

**CMSE4604**

# Dynamic Responses of Electrical, Dielectric and Magnetic Properties of La Substituted Ni-Cu-Cd Bulk Ceramics with Theoretical Justifications

M. Faishal Mahmood and M. Belal Hossen*
*Department of Physics, Chittagong University of Engineering and Technology, Bangladesh*

**Abstract.** Bulk ceramics are needed in many electronic applications instead of powder with controlled grain to reduce pores. It is one of the most valuable objectives for preparing dense ferrites from nanocrystalline powders. It is revealed in many previous cases that suitable substitution in ferrites showed improved characteristics like enhance permeability and resistivity, reduce dielectric loss etc. In the present research shares experience by depicting structural properties along with magnetic and electrical behaviors of $Ni_{0.7}Cu_{0.2}Cd_{0.3}Fe_{2-x}La_xO_4$ dense ceramics synthesized from nanocrystalline ferrites. Analyzing XRD data, the structure of every composition comply with the cubic spinel structure. By the implementation of XRD data, structures have been analyzed through Rietveld refinement technique using Fullprof suite software. After getting good chi2 value different parameters have been determined. These include crystallite size, cation distribution, and electron density. Moreover, Maximum Entropy Map (MEM) has been analyzed for each of every set. In addition bond structures are found by using the output of Rietveld refinement procedure. It is depicted from electric modulus study that dielectric loss tangent reduces exponentially with increasing frequency and remains constant at higher frequency. In contrast, the permeability of dense ceramics is greater for the substitution of Lanthanum ions on ferrites. With the arisen frequency the imaginary part of complex initial permeability decreases linearly while the real part of permeability remains almost constant. The relative quality factor shows the peaking behavior. Dielectric and magnetic properties are justified by the theoretical fitted curves such as NMDE and LAS respectively.

**Keywords:** La-substituted NiCuCd bulk ceramics, Rietveld Refinement, MEM, Dielectric loss tangent, Initial permeability

## Oral Session 2: Characterization and Testing

**Time: 14:00-17:40, August 2, 2021.** Eastern European Summer Time.

**Session Chair: Dr. Marianna Marciszko-Wiąckowska, AGH University of Science and Technology, Poland**

**Session Chair: Mr. Stefan Siebert, Brockhaus Measurements, Germany**

***Session Room Link: http://www.academicconf.com/teamslink?confname=cmse2021***

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| 14:00-14:15 **CMSE4545** | Influence of Sample Orientations on Wrinkle Reduction During the Diaphragm-Forming Process<br>*Dr. Hassan Alshahrani, Department of Mechanical Engineering, Najran University, Saudi Arabia* |
| 14:15-14:40 **CMSE4512** | Microstructures Design in MgO-$SiO_2$-$Al_2O_3$ System by Means of T-x-y Diagram 3D Computer Model<br>*Prof. Vasily Lutsyk, Institute of Physical Materials Science, Siberian Branch of the Russian Academy of sciences, Russian Federation* |
| 14:40-15:05 **CMSE4536** | A New Simple, Highly Sensitive and Selective Spectrofluorimetric Method for the Speciation of Thallium at Pico-trace Levels in Various Complex Matrices Using N-(pyridin-2-yl)-quinoline-2-carbothioamide<br>*Prof. M. Jamaluddin Ahmed, Department of Chemistry, University of Chittagong, Bangladesh* |
| 15:05-15:20 **CMSE4549** | Fatigue Detection and Analysis of Drilling Tools Based on Metal Magnetic Memory Method<br>*Dr. Jingwei Zhang, College of Safety and Ocean Engineering, China University of Petroleum(Beijing), China* |
| 15:20-15:35 **CMSE4563** | Assessment of Stress Distribution in Premium Connections with Ultrasonic Phased Array and Metal Magnetic Memory<br>*Ms. Ting Han, College of Safety and Ocean Engineering, China University of Petroleum, China* |
| 15:35-15:50 **CMSE4474** | Study of Internal Porous Structure Formation of the Powder Metallurgically Prepared Aluminium Foam<br>*Mr. Arun Gopinathan, Institute of Materials & Machine Mechanics, Slovak Academy of Sciences, Slovakia* |
| 15:50-16:00 | **BREAK** |
| 16:00-16:15 **CMSE4540** | Multireflection Grazing Incidence X-ray diffraction (MGIXD) - a New Way of Experimental Data Analysis<br>*Dr. Marianna Marciszko-Wiąckowska, Academic Centre for Materials and Nanotechnology, AGH University of Science and Technology in Krakow, Poland* |
| 16:15-16:30 **CMSE4541** | Stress Anisotropy and Relaxation of Liquid Under Nanoscale Confinement<br>*Dr. Hongyu Gao, Department of Materials Science and Materials Engineering, Universität des Saarlandes, Germany* |

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| 16:30-16:45 | **CMSE4565** | Hydrolysis of Molten $ZnCl_2$-NaCl-KCl and Effect of Adding ZnO<br>*Dr. Sepideh Niazi, Faculty of science and technology, Norwegian University of Life Science (NMBU), Norway* |
| 16:45-17:00 | **CMSE4517** | Synergetic Effect of Metal Sulfides and ZDDP on the Lubricating Performance of a PAO Oil<br>*Dr. Germán Prieto, Engineering Department, Universidad Nacional del Sur, Argentina* |
| 17:00-17:15 | **CMSE4576** | Wavelength Detection Method Using Vortices<br>*Dr. Bruno Saucedo Orozco, Centro de Investigaciones en Óptica, A.C., Mexico* |
| 17:15-17:40 | **CMSE4471** | Advanced Continuous Loss Measurement during Electrical Steel Production<br>*Mr. Stefan Siebert, Brockhaus Measurements, Germany* |

# Abstracts of Session 2

**CMSE4545**

**Influence of Sample Orientations on Wrinkle Reduction During the Diaphragm-Forming Process**

Hassan Alshahrani
*Department of Mechanical Engineering, Najran University, King Abdulaziz Road, P.O Box 1988, Najran, Saudi Arabia*

**Abstract.** Determining wrinkle defects during the diaphragm-forming process is essential to reach acceptable free-defect composite parts for many sectors. The nature of the reinforcement used in forming process plays an important role in terms of wrinkle reduction. In this study, the formability of out-of-autoclave 5-harness satin woven carbon/epoxy prepregs over L-shaped tool was examined using a custom-made diaphragm forming set-up. The relationship between bending stiffness and formed parts was explained in terms of observed wrinkles, processing temperature, and alignment direction to the forming tool. The results showed that alignment of the warp direction to the tool (forming direction) during the diaphragm-forming process is facilitated wrinkle reduction. The different forming results between warp and weft directions indicate that the pre-forming state should be taken into consideration during forming process to achieve the desired shape without defects. However, different shapes with double highly curved should be examined to confirm this drawn conclusion.

**Keywords:** Diaphragm forming, Wrinkling, Out-of-autoclave prepreg, Reinforcement.

**CMSE4512**

**Microstructures Design in MgO-$SiO_2$-$Al_2O_3$ System by Means of T-x-y Diagram 3D Computer Model**

Zelenaya A.E., Lamueva M.V., Lutsyk V.I.*
*Institute of Physical Materials Science, Siberian Branch of the Russian Academy of sciences, Russian Federation*

**Abstract.** A computer model of the T–x–y diagram of MgO–$SiO_2$–$Al_2O_3$ system is used to show the possibility of analysis of its microstructure constitution in terms of competition between primary and eutectic crystals by means of vertical mass balance diagrams calculated for a given centroid over the whole temperature range. The usefulness of horizontal mass balance diagrams is considered for studying phase relations at a fixed temperature along the chosen isopleth. Mass balances were used to determine the crystallization path at the quasi-peritectic liquidus point with the invariant reaction L + $Al_2O_3$ = $3Al_2O_3$ • $2SiO_2$ + MgO • $Al_2O_3$, whose composition was taken into account in giving a rationale to corundum armor element technology. Thus, not only do developed models make it possible to visualize the geometry of a phase diagram, but they are a source of information on crystallization and microstructure formation stages, making it possible to qualitatively and quantitatively evaluate phase ratios and phase assemblage ratios for a given composition.

**Keywords:** Phase diagram, 3D computer model, Microstructure design, Concentration domain, Material genome.

**Acknowledgements:** It has been performed under the program of fundamental research SB RAS (project 0270-2021-0002) and was partially supported by the Russian Foundation for Basic Research (project 19-38-90035).

**CMSE4536**

## A New Simple, Highly Sensitive and Selective Spectrofluorimetric Method for the Speciation of Thallium at Pico-trace Levels in Various Complex Matrices Using N-(pyridin-2-yl)-quinoline-2-carbothioamide

M. Jamaluddin Ahmed
*Department of Chemistry, University of Chittagong, Chittagong-4331, Bangladesh*

**Abstract.** A new spectrofluorimetric reagent N-(pyridin-2-yl)-quinoline-2-carbothioamide (PTQA) has been synthesized and characterized for the speciation of thallium. A very simple, ultra-sensitive and highly selective non-extractive new spectrofluorimetric method for the determination of $Tl^{I}$ and $Tl^{III}$ individually and for mixtures of both analytes at pico-trace levels using N-(pyridin-2-yl)-quinoline-2-carbothioamide (PTQA) has been developed. PTQA has been proposed as a new analytical reagent for the direct non-extractive spectrofluorimetric determination of $Tl^{III}$. This novel fluorimetric reagent, PTQA becomes oxidized in a slightly acidic (0.0025-0.05 M $H_2SO_4$) solution with in $Tl^{III}$ in 20% ethanol to produce highly fluorescent oxidized product ($\lambda_{ex}$ = 324 nm; $\lambda_{em}$= 379 nm). The determination of $Tl^{I}$ is based on the rapid oxidation of this ion by bromine water heating for 15-min with the concomitant formation of fluorescent $Tl^{III}$ - PTQA. Constant and maximum fluorescence intensities were observed over a wide range of acidity (0.0025-0.05 M $H_2SO_4$) for the period between 2 min and 24 h. Linear calibration graphs were obtained for 0.001 – 600-$\mu gL^{-1}$ of thallium, having a detection limit of 0.16-$ngL^{-1}$; the quantification limit of the reaction system was found to be 1.6-$ngL^{-1}$ and the RSD was 0-2%. A large excess of over 60 cations, anions and complexing agents (like, chloride, phosphate, azide, tartrate, oxalate, $SCN^{-}$ etc.) do not interfere in the determination. The developed method was successfully used in the determination of thallium in several Certified Reference Materials (alloys, steels, serum, bovine liver, drinking water, soil and sediments) as well as in some environmental waters (potable and polluted), biological fluids (human blood, urine, hair and milk), soil samples and food samples (vegetables, rice and wheat) solutions containing both $Tl^{I}$ and $Tl^{III}$ and complex. The results of the proposed method for assessing biological, food, soil, water and vegetables samples were comparable with ICP-OES, ICP-MS and AAS were found to be in excellent agreement.

**Keywords:** Spectrofluorimetry, Thallium determination, N-(pyridin-2-yl)-quinoline-2-carbothioamide, Various complex matrices.

**CMSE4549 To avoid repeatability issues, this abstract will be available after the full paper is published in the conference proceedings.**

**CMSE4563 To avoid repeatability issues, this abstract will be available after the full paper is published in the conference proceedings.**

**CMSE4474 To avoid repeatability issues, this abstract will be available after the full paper is published in the conference proceedings.**

**CMSE4540**

## Multireflection Grazing Incidence X-ray diffraction (MGIXD) - a New Way of Experimental Data Analysis

Marianna Marciszko-Wiąckowska
*Academic Centre for Materials and Nanotechnology, AGH University of Science and Technology in Krakow, Poland*

**Abstract.** Experimental data obtained using MGIXD measurements for Ni and austenitic stainless steel, exhibiting significant elastic anisotropy of crystals, were analyzed using different ways of biaxial stress and lattice parameter determination. In the first approach, the calculations were performed using the least square method. Next, two simplified procedures based on the linear regression (weighted and non-weighted) were applied. It was found that all the tested methods give similar results, i.e., almost equal values of the determined stresses, lattice parameter as well as the uncertainties of their determination. The advantage of the newly proposed analyses based on linear regression is their simplicity and straightforward interpretation enabling easy verification of the assumptions concerning grains interaction, texture, and the presence of shear stresses.

**Keywords:** Residual stress, Nickel, Austenitic stainless steel, Elastic anisotropy.

**CMSE4541**

## Stress Anisotropy and Relaxation of Liquid Under Nanoscale Confinement

Hongyu Gao
*Department of Materials Science and Materials Engineering, Universität des Saarlandes, Germany*

**Abstract.** When liquids are squeezed out between two solid surfaces, they often exhibit layering, load-bearing ability, and a much increased viscosity. The combination of these phenomena is frequently interpreted as confinement-induced solidification. Here we propose that such behavior may often better be rationalized as the non-zero wavevector response of a pressurized liquid: bulk liquids contain structure even beyond the nanoscale as evidenced by their (damped) sinusoidal density correlations. Under confinement, this structure enables liquids to sustain non-isotropic stresses and thereby to carry

load over a time span that is long enough for molecules to rearrange in the confined zone. In response to the load, viscosity can increase locally, in which case liquid flow is suppressed. This interpretation is supported by molecular dynamics simulations of a key commercial base-oil component (1-decene trimer), which is squeezed out between a ridge and a substrate. The layering of the oil reflects the density correlations of the bulk liquid. At the same time, the confined liquid can sustain von Mises stresses exceeding locally 100 MPa over sufficiently long times for molecules to diffuse within the confined zone.

**Keywords:** Liquids, Confinement, Tribology, Molecular-dynamics.

**CMSE4565**
**Hydrolysis of Molten $ZnCl_2$-NaCl-KCl and Effect of Adding ZnO**

Sepideh Niazi*, Espen Olsen and Heidi S. Nygård
*Faculty of science and technology, Norwegian University of Life Science (NMBU), Norway*

**Abstract.** Molten salt technology has been used in various applications since the nineteenth century. Their transport and thermodynamic properties make them a proper candidate as a liquefier, solvent and transfer medium for different purposes. One of many possible applications is as biomass liquefier. Liquefaction of biomass using a molten salt makes it pumpable and easily transferable to conversion of biomass to e.g. bio-oil. The selected molten salt needs to have a relatively low melting point. It needs to be low enough to avoid producing ash or char. The molten salt requires high thermal stability to avoid salt decomposition at high temperature and make salt recycling possible. It also needs to have a low hydrolysis rate. Water in biomass may react with the salts and form highly corrosive gases. Therefore, minimizing the rate of hydrolysis is a considerable issue for this study. $ZnCl_2$:KCl:NaCl is a promising molten salt with relatively low melting point, high thermal stability and good properties in contact with biomass. Four compositions of $ZnCl_2$:KCl:NaCl including salt #1: 60:20:20, salt #2: 59.5:21.9:18.6, salt #3: 52.9:33.7:13.4 and salt #4: 44.3:41.9:13.8 in mole fraction are investigated. Salt #4 seems to have the most promising properties, with a relatively low melting point (~205°C), the highest stability (~0.2% mass loss at 500°C) and the lowest HCl concentrations during hydrolysis experiments. Salt #1 had the highest hydrolysis rate. However, addition of ZnO showed a marked, limiting effect on the hydrolysis, especially at temperatures below 400 °C.

**Keywords:** Molten salt, $ZnCl_2$:NaCl:KCl, Hydrolysis, Eutectics.

**CMSE4517**
**Synergetic Effect of Metal Sulfides and ZDDP on the Lubricating Performance of a PAO Oil**

G. Prieto[1,2*], J. Dennehy[1], W. R. Tuckart[1,2]
[1]*Engineering Department, Universidad Nacional del Sur, Argentina*
[2]*IFISUR, Universidad Nacional del Sur/CONICET, Argentina*

**Abstract.** The current trend of increasing the power density of machinery and equipment implies a challenge for lubricating oils, mainly due to the increase in operating temperatures and contact stresses.

To address this scenario, lubricating oils are additivated with compounds that protect the surfaces from direct metal-to-metal contact in boundary lubrication regimes. For this purpose, additives such as zinc dialkyldithiophosphate (ZDDP) have been traditionally used, thanks to their ability to form protective films on steel surfaces. Similarly, metal sulfides such as $MoS_2$ and $Bi_2S_3$ can effectively reduce friction and wear by forming chemically bound layers to steel substrates. However, the joint action of metal sulfides and ZDDP has not been yet fully characterized.

In this work, a PAO ISO VG 6 base oil was additivated with different combinations of ZDDP, $MoS_2$, and $Bi_2S_3$. The formulated oils were tested using a Reichert test (Contact stress: 1.2 GPa; sliding speed: 1.7 m/s; sliding distance: 408 m). Both the fixed cylinder and the rotating ring in the Reichert test were made of AISI 52100 steel with a hardness of 62 HRC. During the tests, the friction force was continuously measured and the wear volume was determined using laser confocal microscopy. Wear scars were also characterized by employing Raman spectroscopy and SEM-EDS microscopy.

The results have shown a strong synergetic effect between ZDDP and both metal sulfides, with a reduction in the wear volume ranging between 31 to 68% in comparison to each of the compounds tested separately.

**Keywords:** $Bi_2S_3$, $MoS_2$, ZDDP, Synergy, Wear, Friction, Lubricating oil.

**CMSE4576**
**Wavelength Detection Method Using Vortices**

Bruno Saucedo Orozco
*Centro de Investigaciones en Óptica, A.C., Mexico*

**Abstract.** An optical system is proposed for wavelength measurement and detection using phase vortices produced by an integrating glass disc. This optical system is based on a modified digital holographic configuration used previously for measurement in Particle Image Velocimetry (PIV) but adapted here for the detection of phase vortices generated by an integrating glass disc. Phase vortices are detected from speckle patterns that are produced using a tunable light with a wavelength of 632 ± 2 nm emitted by a Littrow monolithic tunable external cavity laser, and after multiple reflections in the integrating disc combined with a reference beam and a speckle interferogram is obtained that recorded by a CCD camera. The Fourier transform method is used for speckle phase generated in the proposed optical configuration and analyzed with a vortex detection method that produces a singularities pattern for each wavelength.

**Keywords:** Speckle, Interferogram, Digital holography, Wavelength detection, Vortices, Integrating glass disc, Vortex detection and phase vortex.

**CMSE4471** *Abstract is not showed here.

## Oral Session 3: Mechanical Properties

**Time: 08:30-11:00, August 3, 2021.** Eastern European Summer Time.
**Session Chair: Dr. P.E. Markovsky, G.V. Kurdyumov Institute for Metal Physics, N.A.S. Ukraine.**
***Session Room Link: http://www.academicconf.com/teamslink?confname=cmse2021***

| | | |
|---|---|---|
| 08:30-08:55 | **CMSE4475** | Mechanical Behavior of Titanium Based Composites Reinforced with TiC and TiB Particles Under Quasi-Static and High Strain Rate Compression<br>*Dr. P.E. Markovsky, G.V. Kurdyumov Institute for Metal Physics of N.A.S. of Ukraine, Ukraine* |
| 08:55-09:20 | **CMSE4486** | Partial Slip Texture Configuration Analysis in Slider and Journal Bearings<br>*Prof. T. V. V. L. N Rao, Department of Mechanical-Mechatronics Engineering, The LNM Institute of Information Technology, India* |
| 09:20-09:35 | **CMSE4573** | Process Analysis of Weld Bond Joint for Tensile Strength and Peel Strength of Dissimilar Ferrous Alloy<br>*Dr. Lokesh Kumar Boriwal, Department of Mechanical Engineering, SAGE University, India* |
| 09:35-10:00 | **CMSE4467** | Experimental and Numerical Studies on Vibration of Laminated Composite Beam with Transverse Multiple Cracks<br>*Dr. Shishir Kumar Sahu, Department of Civil Engineering, National Institute of Technology, Rourkela, India* |
| 10:00-10:20 | | **BREAK** |
| 10:20-10:35 | **CMSE4597** | Development of Ideal Processing Parameters for Powder Bed Fusion System Processing of AlSi10Mg using Design of Experiments<br>*Dr. Ntombizodwa R. Mathe, Laser Enabled Manufacturing Research Group, National Laser Centre, Council for Scientific and Industrial Research, South Africa* |
| 10:35-11:00 | **CMSE4612** | Casting Layout Design Using CAE Simulation with Household Appliance (Cooking Grill)<br>*Assoc. Prof. Hong-Kyu Kwon, Dept. of Industrial and Management Engineering, Namseoul University, South Korea* |

# Abstracts of Session 3

**CMSE4475**

**Mechanical Behavior of Titanium Based Composites Reinforced with TiC and TiB Particles Under Quasi-Static and High Strain Rate Compression**

P.E. Markovsky[1*], J. Janiszewski[2], O.O. Stasyuk[1], V.I. Bondarchuk[1], D.G. Savvakin[1], K. Cieplak[2], P. Dziewit[2], S.V. Prikhodko[3]

[1]*G.V. Kurdyumov Institute for Metal Physics of N.A.S. of Ukraine, 36, Vernadsky Blvd., 03412, Kyiv, Ukraine*

[2] *Jarosław Dąbrowski Military University of Technology, 2, gen. Sylwester Kaliski str., 00 – 908 Warsaw 46, Poland*

[3]*University of California, Los-Angeles, Department of Materials Science and Engineering, Los Angeles, CA 90095, USA*

**Abstract.** Mechanical behavior of titanium alloy Ti-6Al-4V and metal matrix composites (MMC) on its base reinforced with TiC and TiB particles were studied under quasi-static and high strain rate compression. The alloy and composites with 5, 10, and 20 % (vol.) of reinforcement were fabricated using blended elemental powder metallurgy. High strain rate compression within the range of 1100÷3350 $s^{-1}$ was accomplished using split Hopkinson pressure bar method. For comparison, these materials were also subjected to standard quasi-static compression tests with strain rate of $10^{-3}$ $s^{-1}$. The true stress – true strain curves were analyzed in terms of the strain rate, phase composition and microstructure, as well as strain energy values. It was shown that at the strain rates up to 1920 $s^{-1}$ TiC composite with 5% of the particles content was characterized with increase of the strength and strain energy values when compared to conventional cast and wrought Ti-6Al-4V alloy. It was established that the presence of 5 to 10% TiC particles in MMCs causes the localization of plastic deformation at the micro-level and plays significant role in deformation mechanism. The fracture is mainly occurred due to the crushing of relatively coarse TiC particles and their aggregates, while titanium matrix deformed plastically. The composites structures significantly weaken with the increase of the particles content up to 20%. Carbide particles remain the weakest microstructural elements which resulted in increased embrittlement of MMCs and their fracturing at low rates (less than 1500 $s^{-1}$) due to simultaneous crushing of carbide particles and formation of the cracks in the matrix between them. MMCs' strengthened with TiB are characterized with lower strength and strain energy values compared to TiC composites with the same amount of reinforcement particles. However, TiB composites demonstrate better ductility characteristics and as a consequence they do not break at strain rates up to 3000 $s^{-1}$.

**Keywords:** Titanium alloys and metal matrix composites, Strain rate, Phase composition, Microstructure, Mechanical characteristics.

**CMSE4486**
**Partial Slip Texture Configuration Analysis in Slider and Journal Bearings**

T. V. V. L. N Rao
*Department of Mechanical-Mechatronics Engineering, The LNM Institute of Information Technology, India*

**Abstract.** There has been widespread interest in partial slip and texture configuration analysis in fluid film bearings. It has been recognized that the tribological performances of high-speed sliding surfaces are modified with partial extent of slip and textures. The performance of slider and journal bearings are enhanced in terms of improvement in load capacity and reduction in coefficient of friction. The partial slip texture designs aimed at providing the desired performance of the fluid film bearings are discussed.

**CMSE4573**
**Process Analysis of Weld Bond Joint for Tensile Strength and Peel Strength of Dissimilar Ferrous Alloy**

Lokesh Kumar Boriwal
*Department of Mechanical Engineering, SAGE University, India*

**Abstract.** Evaluating the strength performance of spot welded joints in dissimilar material is critical for their continued addition into the automobile and aerospace industries. The effect of weld joint strength is an important attention in the design of structures. The aim of this paper is to estimate the effect of the welding process parameters (welding current, weld time, and electrode pressure) on the mechanical performance of dissimilar weld bonds between austenitic stainless steel 304L and low carbon steel sheets. Mechanical properties of weld bonds are defined in terms of weld bond strength, failure mode, and hardness of the joint. Weld bonding experiments were planned on the basis of FFD. Weld bonded joint strength assessments exhibited that the maximum tensile shear strength and peel strength were achieved at 6.4 kA, eight-cycle weld time with 3 kg/cm2 electrode pressure. The hardness value across the weld bonded fusion zone was not affected much with respect to varying the welding current. Pullout failure and tearing failure modes were observed during the tensile shear strength test of weld bonded joints. Application of adhesive layer at faying surfaces resulted not only in strengthening but also distributing the stress in weld bonded joints.

**Keywords:** Weld bonding, tensile shear strength, peel strength, mechanical properties

**CMSE4467**

# Experimental and Numerical Studies on Vibration of Laminated Composite Beam with Transverse Multiple Cracks

S K Sahu[1,*] and P Das[1,2]
[1]*Department of Civil Engineering, National Institute of Technology, Rourkela, India*
[2]*Department Civil Engineering, ITER, SOA University, India*

**Abstract.** Composite beams are increasingly used in aerospace, automobile and other applications. Crack is the most common defect in structures during its service life. The cracked composite beams are subjected to dynamic loads and the vibration of the cracked beams is of technical significance to the structural integrity of systems. The objective of the present investigation is to demonstrate the vibration characteristics of laminated composite beams (LCB) with multiple transverse cracks. Finite element method (FEM) is used for the frequency-based crack analysis in this study. A computer program is developed in MATLAB environment for numerical analysis. First-order shear deformation theory (FSDT) is adopted for the numerical analysis. Composite specimens are casted using hand lay-up technique and are tested for its material constants under tensile test. Experiments are conducted using woven roving. Glass/Epoxy laminated beam samples with pre-defined cracks. The obtained test results from the experimental work using FFT analyzer are validated with the numerical results obtained through MATLAB. The effects of natural frequencies with respect to the various boundary conditions, crack depth and locations are investigated to support in real applications. A fine agreement is accomplished between the numerical and test results. Both the studies showed that natural frequencies in the LCB are significantly influenced by the location and size of the cracks. The results show that natural frequencies are decreased with cracks and an increase in
fiber orientations of composite cracked beams.

**Keywords:** Laminated composite beam, Vibration, Cracks, Finite element method, FFT analyser.

**CMSE4597**

**Development of Ideal Processing Parameters for Powder Bed Fusion System Processing of AlSi10Mg using Design of Experiments**

Ntombizodwa R. Mathe
*Laser Enabled Manufacturing Research Group, National Laser Centre, Council for Scientific and Industrial Research, Pretoria, South Africa*

**Abstract.** The additive manufacturing of aluminium alloys have gained great interest in the transport industry in the past 10 years. This is mainly due to the light weight and good strength that these alloys offer especially for applications in the aerospace and other related industries. However, there are drawback in using these alloys especially the parts produced by additive manufacturing as they have to be heat treated before application to relieve residual stresses caused by the fast heating and cooling experienced during powder bed fusion (PBF) fabrication. Most of the current PBF metal system offer a variety of processing parameters for part building, however AM uptake and industrial implementation is still slow due to restrictions of the laser power and scanning speed that are slow and thus the parts take long to produce. Seeing this lag in the market, the CSIR has produced a high speed and high power PBF machine with a build platform larger than the currently available commercial systems. This system allows for the faster production of parts due to its higher consolidation rate and it has already been validated for aluminium alloys, specifically AlSi10Mg. The properties evaluated were microstructure and hardness, which found to be comparable to commercial PBF machines. The samples were analysed for microstructure, mechanical properties using tensile and nano indentation procedures.

The aim of this work is to develop process specifications on the CSIR-built PBF for AlSi10Mg starting with process optimization, part building/prototyping and post processing for the fulfillment of the AM value chain.

**Keywords:** Additive manufacturing, Powder bed fusion, AlSi10Mg, Nano-indentation.

**CMSE4612**

**Casting Layout Design Using CAE Simulation with Household Appliance (Cooking Grill)**

Hong-Kyu Kwon
*Dept. of Industrial and Management Engineering, Namseoul University, South Korea*

**Abstract.** Due to the development and industrialization of science and technology, the use of aluminum alloys has been developed in various fields. Recently, the government is pursuing lightweight and recyclability of various components due to resource and energy conservation and environmental problems. In the foundry industry, products using cast iron are being replaced by aluminum products using high-pressure die casting (HPDC) in parallel with this trend. Casting layout design, which relies on the experience and know-how of mold designers in the casting industry, was insufficient to respond to the rapidly changing needs of the era and increase production costs. Designing casting layout using CAD/CAM/CAE technology and producing casting layouts have become critical issues.

Computer-Aided Engineering (CAE) technology is rapidly increasing with the development of computer software and hardware. CAE technology not only predicts defects in mass production but also performs filling or solidification analysis during the mold design stage before production, enabling optimal mold design methods. New technologies that combine the casting process of filling and solidification analysis with computer simulation and field technology using practical know-how are rapidly increasing in the foundry industry.

Based on empirical know-how, the casting layout design of casting products was used through trial and error. The solution achieved through the scientific calculation and analysis of CAE technology saves a lot of money and time to build die-casting molds and applies to the design and fabrication of die-casting molds. In this study, numerical analysis of household appliances (cooking grill) quickly and accurately predicts problems arising from the filling and solidification of the melted metal in the casting process, thereby preventing the casting products' quality. These results are used to establish a sound casting layout quickly, along with reducing production costs.

**Keywords:** Cooking grill, Gate system, High-pressure die-casting, CAE simulation, Flow analysis.

**Acknowledgements:** Funding for this paper was provided by Namseoul University.

## Oral Session 4: Metals, Ceramics, Composites, Polymers

**Time: 13:30-18:05, August 3, 2021.** Eastern European Summer Time
**Session Chair: Dr. Yanli Lu, Northwestern Polytechnical University, China**
***Session Room Link: http://www.academicconf.com/teamslink?confname=cmse2021***

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| 13:30-13:55 **CMSE4546** | The Relationship Between the Annealing Cycle and the Magnitude of the Recovered Enthalpy for Glass Transition in Polystyrene<br>*Dr. Yutaka Tanaka, Department of Materials Science and Biotechnologies, School of Engineering, University of Fukui, Japan* |
| 13:55-14:10 **CMSE4535** | Solid Oxide Fuel Cells: Synthesis and Degradation Study of Na-doped $SrSiO_3$ Solid Electrolyte<br>*Dr. Kapil Sood, Department of Physics, Dr. S. Radhakrishnan Government Degree College Dharampur, India* |
| 14:10-14:35 **CMSE4618** | Phase Field Crystal Study of the Grain Boundary Segregation and Grain Boundary Premelting in Binary Alloy<br>*Dr. Yanli Lu, State Key Lab of Solidification Processing, Northwestern Polytechnical University, China* |
| 14:35-14:50 **CMSE4555** | High Entropic Metal, Nitride, Oxide and Carbide Coatings<br>*Dr. Viacheslav Stolbovyi, National Academy of Sciences of Ukraine / National Scientific Center "Kharkov Institute of Physics and Technology", Ukraine* |
| 14:50-15:05 **CMSE4529** | Polyamide Membrane Preparation: A Review<br>*Dr. Ayman El-Gendi, Chemical Engineering & Pilot Plant Department, Engineering Research Division, National Research Centre, Egypt* |
| 15:05-15:30 **CMSE4460** | Reliability and Maintenance of Large Wind Turbine Blades: Materials Science Aspects<br>*Dr. Leon Mishnaevsky Jr., Department of Wind Energy, Technical University of Denmark, Denmark* |
| 15:30-15:55 **CMSE4504** | Anodic Surface Modification of Titanium and Its Alloys: Crucial Aspects for Biomedical Applications<br>*Dr. Anca Mazare, Department of Materials Science – WW4-LKO, Friedrich-Alexander University of Erlangen Nurnberg, Germany* |
| 15:55-16:10 | **BREAK** |
| 16:10-16:25 **CMSE4478** | Be Green, Be Smart<br>*Dr. Sumita Goswami, Almascience, CoLAB, Caparica, Portugal* |
| 16:25-16:50 **CMSE4574** | A Role of the Perovskite Lattice Vacancies in Antiferrodistortive Phase Transition of Doped Strontium Titanate Ceramics<br>*Dr. Oleksandr Tkach, CICECO – Aveiro Institute of Materials, Department of Materials and Ceramic Engineering, University of Aveiro, Portugal* |
| 16:50-17:05 **CMSE4538** | Surfaces Modification of Ti15Mo by YSZ Coating Deposition by PS-PVD Method for Medical Application<br>*PhD Jagoda Barczyk, Institute of Materials Science, University of Silesia in Katowice, Poland* |

| | |
|---|---|
| 17:05-17:20 **CMSE4581** | Oxygen Plasma Treatment Effects on Polymeric Membranes Loaded with Felodipine<br>*Dr. Maraolina Domínguez-Díaz, Centro de Investigación y de Estudios Avanzados del Instituto Politécnico Nacional Unidad Saltillo, Mexcio* |
| 17:20-17:35 **CMSE4539** | Studies on Mechanical & Thermal Properties of Polypropylene/ Polyolefin elastomer/Epoxidized Soyabean Oil/Sepiolite Composites<br>*Mr. Rushikesh Vilas Kumbhakarna, School of Polymer Engineering, Dr. Vishwanath Karad MIT World Peace University, India* |
| 17:35-17:50 **CMSE4543** | PBAT/PBS/HNT Filled Blends for Active Food Packaging<br>*Ms. Prachi Desai, School of Polymer Engineering, Dr Vishwanath Karad, MIT World Peace University, Pune, 411 038, India* |
| 17:50-18:05 **CMSE4566** | Multi-criteria Selection of Hybrid Alkaline-Activated Cementitious Binders for the Potential Production of Ceramic Composites<br>*Mr. Andrés Valencia Isaza, Grupo de Investigación en Materiales Alternativos y Procesos Automáticos (MAPA), Universidad EIA, Colombia* |

# Abstracts of Session 4

**CMSE4546**

## The Relationship Between the Annealing Cycle and the Magnitude of the Recovered Enthalpy for Glass Transition in Polystyrene

Y. Tanaka*, N. Sakamoto
*Department of Materials Science and Biotechnologies, School of Engineering, University of Fukui, Japan*

**Abstract.** Sub-$T_g$ ageing is a thermodynamic phenomenon involving volume and enthalpy relaxation upon annealing below the glass transition temperature ($T_g$) for a glassy polymer, which causes changes in physical/mechanical properties. The nature of these changes is a slow evolution toward equilibrium by losing the excess thermodynamic quantity. This phenomenon, referred to as physical ageing and/or structural relaxation, brings about an alteration of the engineering properties of plastics, and thus may result in technological troubles. In starting the ageing study for conventional polymeric materials, the enthalpy relaxation experiments were conducted for polystyrene samples at different annealing temperatures below $T_g$ with the method of differential scanning calorimetry. The framework of Tool-Narayanaswamy-Moynihan approach was applied to reproduce experimental traces with two models of the relaxation times; those are the generalized Arrhenius form which combines the real temperature and the fictive temperature ($T_f$ model) dependences, and the config-urational entropic form ($S_c$ model). The calculation data of the heat capacity ($c_p$) obtained from the two models were analysed on the basis of the parameter – geometry relationship, in which three factors were given to the geometry of the $T_g$ shoulder and overshoot appeared in $c_p$ curve. The comparison between experimental and the calculation $c_p$ data showed no significant differences. It was found that both the horizontal shift and the broadening of $T_g$ shoulder occur interdependently in the $c_p$ curve calculation of $S_c$ model, while they are almost independent in the calculation of $T_f$ model. The series operations for the calculation $c_p$ data to simulate the experimental data were followed in part regarding the $T_f$ model. In addition, the analysis revealed the process of producing $c_p$ overshoot in $T_g$ shoulder, which is expected to be instructive in the optimized $c_p$ calculation for the experiment of the effect of stretching on physical ageing.

**Keywords:** Glass transition, Enthalpy relaxation, Cooperative rearranging, Polystyrene, Physical ageing.

**CMSE4535**

## Solid Oxide Fuel Cells: Synthesis and Degradation Study of Na-doped $SrSiO_3$ Solid Electrolyte

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**Abstract.** Solid electrolytes are the important class of materials that have received wide attention because of their potential applications viz. solid oxide fuel cells, solid state batteries and as gas sensors. The main challenge in commercialization of these materials is its high operating temperature. Therefore, research focus is on the development of new electrolytes that can possess appreciable conductivity at intermediate temperature (400-600 °C) range. Na-doped $SrSiO_3$ (SNS) is recently reported as promising oxide-ion conductor in the intermediate temperature range. However, its material stability is still a major issue which requires proper investigation. In addition, there are contradictory reports on the ionic conductivity and material stability of SNS by various research groups. So, we have synthesized and systematically investigated the conductivity and stability issues for its use as solid electrolyte.

Keeping in mind aforesaid issues, in the present work, $Sr_{1-x}Na_xSiO_{3-\delta}$ (x=0.0, 0.10, 0.20, 0.30 and 0.40) have been synthesized by solid state reaction method. The phase and morphology of as-prepared samples were investigated by XRD, SEM/EDS, TEM etc. AC impedance spectroscopy is used to study the conductivity of the system. $Sr_{0.6}Na_{0.4}SiO_{3-\delta}$ showed highest conductivity ~0.02 S/cm at 800 °C in air. Ion transport study is performed to find the type of charge carriers responsible for conductivity in this system. The material degradation study is also performed on selective samples.

**CMSE4618**

## Phase Field Crystal Study of the Grain Boundary Segregation and Grain Boundary Premelting in Binary Alloy

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**Abstract.** Grain boundary plays an important role in the physical and chemical properties of polycrystalline materials. Grain boundary segregation is a common metallic phenomenon in alloys. Many grain boundary phenomena, such as grain boundary migration, grain boundary sliding, grain boundary corrosion, grain boundary melting, grain boundary strengthening, as well as the strength, fracture, creep resistance, electron transport, corrosion and other behaviors related to these phenomena are related to the segregation of grain boundary elements. The segregation of trace elements at the alloy interface (such as phase boundary and grain boundary) greatly affects the properties of the material, so the study of the segregation law at the interface is of great practical significance.

In this paper, the phase field model of binary alloy was used to study the grain boundary segregation and microstructure evolution during the pre-melting process of binary alloy. The microstructure morphology of grain boundary segregation with different orientation difference angles was simulated. The characteristics of grain boundary segregation and the relationship between grain boundary segregation and temperature, orientation difference Angle, undercooling degree, lattice mismatch degree and interatomic binding energy were analyzed. The variation of the concentration and the structure of grain boundary in the process of grain boundary premelting were studied.

**Keywords:** Binary phase filed crystal, Binary alloy, Grain boundary segregation, Grain boundary premelting, Width of liquid film.

**Acknowledgements:** This work was supported by the National Natural Science Foundation of China (NSFC) (Grant Nos. 51974258, 51674205, 51575452). The author thanks Professor Long-Qing Chen of Pennsylvania State University for his nice discussion and help.

**CMSE4555**
**High Entropic Metal, Nitride, Oxide and Carbide Coatings**

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Abstract. The production of high-entropy coatings was carried out by the method of vacuum-arc deposition in an improved Bulat-6 installation and ion sputtering in the plasma of a compressed vacuum-arc discharge.

The properties of arc coatings are influenced by the preliminary pressure in the chamber during deposition (various gases) and the voltage applied to the substrate, as well as by the material of the high-entropy cathode used.
High-entropy nitride coatings are solid solutions based on an FCC lattice, which are characterized by high hardness. Since all the elements included in their composition have an FCC lattice, this makes it possible to calculate the lattice parameter of high-entropy nitride coatings.

It turned out that for nitride coatings and for cast high-entropy alloys, the determined lattice parameter is larger than the calculated one. At the same time, for nitride coatings, there is a tendency to a decrease in hardness with an increase in the difference between the calculated and determined values of the lattice parameter.

High hardness values provide high-entropy nitride coatings with superior wear resistance over single-component nitrides. High-entropy nitride coatings are characterized by high values of hardness 50 ... 60 GPa, and elastic modulus of more than 500 GPa, and also have thermal stability up to annealing temperatures of 1300 °C in an inert atmosphere.

The hardness of high-entropy carbide (TiZrHfVNbTa)C reaches 43–48 GPa, and the elastic modulus is 480 GPa. Studies of the wear resistance of a high-entropy carbide coating based on the TiZrHfVNbTa alloy showed that the coefficient of friction in a pair with diamond in the load range from 2,2 to 5,5 N varies from 0,09 to 0,104. Investigation of changes in the friction force during reciprocating oscillations of the indenter at a constant load of 100 g. showed that in the process of repeated deformations, the friction coefficient decreases from 0,105 to 0,07.

Oxide coatings based on the AlTiCrVNbMo alloy are characterized by hardness at the level of 30 ... 32 GPa, a high value of the normalized hardness of the order of 0,118 ... 0,133 and the lowest coefficient of friction at the level of 0,045.

**Keywords:** Vacuum arc coatings, High entropy materials, Superhard.

**CMSE4529**
**Polyamide Membrane Preparation: A Review**

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**Abstract.** This article is an overview on the polyamide (PA) membrane preparation, characterization and application. As a matter of fact, the PA membranes are prepared via different techniques such as phase inversion, interfacial polymerization (IP), track-etching, electro-spinning, etc. Additionally, polyamide membrane preparation depends on the required application, which is dependent on the membrane type and its structure. Phase inversion (PI) process and interfacial polymerization (IP) are the most applied methods for preparing polyamide membrane. Whereas the PA membranes are already prepared, a pre-classification depends on its properties occur for using it in the suitable application which is dependent on membrane properties. For that purpose, the polyamide membrane is characterized for defining their properties, such as morphology, surface roughness, and mechanical property, hydrophilic property, swelling degree, contact angle, membrane charge and gel content, which in turn are related to the membrane preparation parameters. From one point, these challenges have the most important influence on polyamide membrane performance, therefore the most important characterization methods for polyamide membrane properties are ascribed to discuss in details. Simultaneously, the applications of polyamide membrane as pressure driven membrane separation processes (PDMSP) are reported.

**Keywords:** Polyamide membrane, Preparation, Characterization, Application, Porous structure, Performance.

**CMSE4460**

## Reliability and Maintenance of Large Wind Turbine Blades: Materials Science Aspects

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**Abstract.** European countries now have 205 GW of wind energy capacity. Wind energy accounted for 15% of the electricity the EU countries, including UK, in 2019. Wind turbines are large structures, which also can be more and more often installed offshore, with rather high costs of maintenance, repair and decommissioning. The requirements toward the wind turbine reliability are therefore very high, as compared with, for instance, automotive structures (where the service points are easily available) or even aerospace structures (which, in the case in aeroplanes, can be daily inspected, without any cost limitations). This sets rather high requirements to the materials, used in wind turbines, in particular, to the wind turbine blades, which are manufactured from lightweight composites, and are permanently moving, subject to complex mechanical and environmental loads. In this presentation, we will discuss several critical materials science related challenges, critical for wind turbine blades. Among these challenges, the problems of erosion and repair of wind turbine blades, protection and maintenance, and perspectives of waste management of composite blades are discussed. The applicability of computational modelling to the optimization of these processes and materials is demonstrated. The materials science solutions for the improving the wind turbine blade reliability, strength and end of life management are reviewed.

**Keywords:** Wind energy, Composites, Maintenance, Renewable energy.

**CMSE4504**

## Anodic Surface Modification of Titanium and Its Alloys: Crucial Aspects for Biomedical Applications

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**Abstract.** Titanium and titanium based alloys are well established as ideal implant biomaterials and moreover tremendous attention was given in the last 20 years to nanoscale surface modifications as it leads to improved biocompatibility and corrosion resistance. Electrochemical anodization is the most widely used method for growing self-organized $TiO_2$ nanostructures, as nanotubes, nanopores, mesoporous, etc. Their widespread use is mostly enabled by the nanoscale topography, large surface area, directional charge and ion transport properties, exclusion effects and defined diffusion behaviour. In regard to biomedical applications, the nanotopography of the surface as well as its high surface are clearly affecting their use in specific applications (such as osseointegration, antibacterial activity, drug delivery, mitigation of the inflammatory response, etc.). From this respect, anodization allows growing of self-organized $TiO_2$ nanotubes directly on the metallic substrate, as well as scalability, adaptability to other substrates such as alloys, and very good control over the nanoscale geometry. Cells react to such nanoscale dimensions and can be synergistically influenced by the nanostructures morphology (e.g. nanotube diameter) and/or by addition of growth factors. Herein we discuss an overview of the

influence of the anodization parameters for obtaining different nanotubular morphologies and their effect on the top morphology of the nanotubes (initiation layer, open-top, nanograss) as well as crucial aspects of nanostructuring via anodization tailored for biomedical applications. In addition we present a very synthetic overview of the effect of such morphologies in view of biomedical applications and their tremendous advantage for further use in biomedical applications.

**Keywords:** Electrochemical anodization, TiO2 nanotubes, Biomedical applications.

**CMSE4478**
**Be Green, Be Smart**

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**Abstract.** Cellulose is the most abundant biomass material on our planet earth. Its salient features like biocompatibility, biodegradability, recyclability, mechanical robustness, lightweight, flexibility and low-cost, have made it a subject matter of immense interest to both academia and industries. In modern world, while we are struggling with the adverse changes in climate due to the ever-increasing burden of carbon-emission from industries, including the huge demands for limited raw materials and hurdles related to growing e-waste amount and its management, we should really channelize all our efforts to think about the plausible solutions and take immediate steps towards sustainable world and circular economy. Paper is one of the major outcomes from cellulose and one of the most important technologies for the existence of mankind with a sustainable future. Recently, its use in some special smart applications like packaging, diagnostics, and security have become quite inevitable. Here in Almascience and CENIMAT we are trying to explore the cellulose beyond paper. Whether it is developing transistors, or paper-on-chip for biological tests, or optoelectronics, or even as a platform for energy harvesters cellulose substrates are being explored vividly and have already shown a lot of potential as an emerging smart candidate for the corresponding applications. Let us use our knowledge and resources to develop Green Technology.

**Keywords:** Cellulose, Paper, Sustainability, Smart Electronics, Green Technology.

**CMSE4574**

## A Role of the Perovskite Lattice Vacancies in Antiferrodistortive Phase Transition of Doped Strontium Titanate Ceramics

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**Abstract.** $SrTiO_3$-based compounds have been attracting considerable interest both for a wide range of applications and from a fundamental point of view. Fundamentally, perovskite-structured $SrTiO_3$ undergoes a cubic (Pm3m) to tetragonal (I4/mcm) phase transition at ~108 K ($T_a$) associated with rotations of the O octahedra in antiphase around the [001] direction. This phase transition gives rise to modes at the R-point of the Brillouin zone. Here, inelastic light scattering as well as electron diffraction are used to study the lattice dynamics of $SrTiO_3$ ceramics with isovalent and heterovalent dopants, substituting for $Sr^{2+}$ or $Ti^{4+}$ ions. Even for a small percentage of Mn or other dopants, $T_a$ is significantly altered, varying oppositely to the tolerance factor ($t$). In the case of sintering $SrTi_{0.95}Mn_{0.05}O_{3-\delta}$ ceramics in $N_2$ or substituting $Ti^{4+}$ with acceptor $Mg^{2+}$ dopant, $T_a$ is strongly suppressed due to a creation of oxygen vacancies, disrupting the octahedra connectivity needed for their cooperative rotation. On the other hand, for Sr-site donor dopants ($La^{3+}$, $Gd^{3+}$, $Y^{3+}$), a common linear dependence of $T_a$ versus $t$ is obtained, if strontium vacancies with a size ~7% larger than $Sr^{2+}$ radius are taken into account.

**Keywords:** Perovkites, Phase transitions, Doping, Vacancies.

**CMSE4538**

## Surfaces Modification of Ti15Mo by YSZ Coating Deposition by PS-PVD Method for Medical Application

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**Abstract.** Recently titanium alloys are widely used in medical area in particular as orthopedic implants. For example, popular materials are Ti-15Zr, Ti-6Al-4V, Ti-6Al-7Nb, Ti-12Mo-3Nb, Ti-15Mo. Because of excellent biocompatibility, mechanical and chemical properties and corrosion resistance. As we know, high biocompatibility of titanium is closely identified with the properties of the alloy surface. Surfaces modification general ensure to allow to selection of optimal roughness, topography and chemistry of implant surfaces. These modifications are intended to improve the binding capacity between the tissue and the implant by increasing the contact surface. In other words, increase osteoconductive properties. Now, the most widely used commercial technique of surface treatment e.g. sol-gel, micro arc oxidation (MAO), Electron Beam Plasma Vapor Deposition (EB-PVD). Many coatings obtained by the mentioned methods show a lot of disadvantages such as delamination,

microcracks, lack of adequate surface for bone cell growth. In this work, decided the modification of surfaces by modern technique Plasma Spray – Physical Vapour Deposioton. Nowadays, widely used in aerospace's industry. The method allowed improved or completely eliminate above mentioned disadvantages of surfaces witch in medicine is unacceptable. Prepared a series of samples with different time of sprayed. The deposited coating surfaces were subjected to GIXD analysis to determine the phase composition of the material. For surface imaging, HR-SEM tests were performed and cracks and coatings were excluded. Furthermore, wear resistance and microhardness tests were carried out. Finally, one of the most important tests was performed in terms of using the material as an implant - surface wettability test.

**CMSE4581**

## Oxygen Plasma Treatment Effects on Polymeric Membranes Loaded with Felodipine

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**Abstract.** Felodipine is one of the most widely used drugs for treating hypertension, which is the leading risk factor for cardiovascular disease. The consumption of this medication can cause adverse reactions, such as headache, dizziness, heartburn, constipation, and enlargement of the gum tissue around the teeth. Currently, much less harmful drug dosage systems for patients can be developed, among which polymer membrane systems. Besides, plasma can be used to control drug release by modifying the surface characteristics of the material without altering its bulk properties. In this work, polyhydroxybutyrate and polyethyleneglycol films and membranes loaded with felodipine were treated with oxygen plasma. The following was evaluated: 1. the release of membrane components during the oxygen plasma treatment, using Optical and Mass Emission Spectroscopies; 2. the effect of the treatment on the polymers and felodipine before and after plasma, employing Raman spectroscopy; 3. the release of felodipine from plasma-treated and untreated materials, through UV-Visible and Raman Spectroscopies. The oxygen plasma can be applied to membranes with felodipine to modulate the dosage of the drug.

**Keywords:** Drug delivery, Plasma, Polymer, Felodipine, Spectroscoy.

**CMSE4539**

# Studies on Mechanical & Thermal Properties of Polypropylene/ Polyolefin elastomer/Epoxidized Soyabean Oil/Sepiolite Composites

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**Abstract.** Polypropylene (PP) has many applications in the field of automobiles due to its good mechanical properties & lower cost. In order to improve the impact strength of polypropylene generally, it is blended with different impact modifiers and maleic anhydride grafted PP as compatibilizer. However, mineral-filled PP requires a different approach. PP filled with sepiolite is a promising material for different applications. In this paper, we studied the effect of 20 wt% Polyolefin elastomer (POE) and 7.5 wt% and 15 wt% Epoxidize soyabean oil (ESBO) as a compatibilizer on various properties of sepiolite–filled PP composites containing 0 to 30% sepiolite filler.

The mechanical and thermal properties of the sepiolite-filled PP compositions were evaluated. The overall mechanical properties of sepiolite-filled PP compositions are essentially decided by the wettability of the filler. It was observed that with the addition of sepiolite, the stiffness increases, and with 20 % POE and 10 % sepiolite filler, there is a significant improvement in impact strength of filled PP composition as compared to virgin PP. Epoxidize soyabean oil also helped to enhance the thermal stability of PP-filled compositions. From Thermogravimetric analysis (TGA) it was observed that the degradation onset temperature shifted considerably (from 336 oC to 343 oC) and weight loss decreased even at 490 oC with the addition of ESBO. The structure development was studied using wide-angle X-ray diffraction (XRD) and the molecular interaction examined using FTIR. XRD data indicated that PP crystals were in α phase but the relative intensities of 110, 040, and 131 reflections changed in presence of sepiolite and ESBO suggesting preferential nucleation/ growth direction of the crystallites. There was also an improvement in crystallinity with the addition of sepiolite. FTIR analysis showed good interaction of sepiolite, ESBO which helped in better compatibility with PP matrix. Thus, by the addition of optimum loading of POE, ESBO in sepiolite-filled PP compositions, there can be significant improvement achieved in impact strength and better thermal stability as compared to virgin PP.

**Keywords:** Polypropylene (PP), Sepiolite, Polyolefin elastomer (POE) & Epoxidized Soyabean Oil (ESBO).

**CMSE4543**
**PBAT/PBS/HNT Filled Blends for Active Food Packaging**

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**Abstract.** Crystalline structure developed in solution cast films of Polybutylene Succinate (PBS) blended with Polybutylene Adipate Co-Terephthalate (PBAT) was studied in detail with respect to composition of the blend. The effect of nanofillers (Halloysite nanotubes/HNT) incorporation as well as addition of polyethylene glycol (PEG) as plasticizer on crystallization process was also investigated. The samples were casted on a glass plate substrate from solution using membrane caster at constant speed and thickness in the range of 100 microns. The composition was varied from 0 to 90 % of PBS in PBAT matrix. Films were air dried in an oven at 50-55 $^{o}$C for 6 hr. The crystal structure development was studied using wide angle X-ray diffraction (XRD), Differential Scanning Calorimetry (DSC) and the molecular interaction examined using FTIR. XRD data indicated that PBS crystals were in monoclinic α phase but the relative intensities of the 011 and 020 reflections changed drastically in the blends. Also new reflections which were not reported earlier were seen distinctly in these blends. PBAT phase also showed crystalline nature with few distinct peaks. The DSC analysis revealed that there were preferential growth of PBS α phase crystals with sharp melting at 110 $^{o}$C. Halloysite nano tubes (HNT) gave distinct nucleation effect with a shift in the temperature of crystallization peak in the DSC cooling curves as well as increase of $\Delta H_c$ value. The preferential nucleation by HNT could be associated with the close lattice match for the HNT and the monoclinic phase of PBS. These changes in the crystallinity and crystal phase improved the barrier properties of the films containing HNT which was seen in the decrease in water vapor transmission rate (WVTR) with the addition of HNT.

**Keywords:** Polybutylene succinate (PBS), Polybutylelne adipate terphalate (PBAT), Halloysite nanotubes, HNT, X-ray diffraction, (XRD), Differential scanning calorimetry (DSC), Water vapor transmission rate (WVTR)

**Acknowledgements:** The authors would also like to acknowledge the support from The Principal, Baburao Gholapji College, Sanghvi, Pune for their help in characterizing samples under XRD. Authors sincerely thanks to the Honorable Director, Prof. (Dr) Vishwanath D Karad, MIT World peace Unversity, Pune for constant encouragement and financial support.

**CMSE4566**

# Multi-criteria Selection of Hybrid Alkaline-Activated Cementitious Binders for the Potential Production of Ceramic Composites

Andrés Valencia Isaza*, José William Restrepo Montoya, Johanna Mercedes Mejía Arcila and Marco Fidel Valencia García

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**Abstract.** In the context of circular economy and adopting one of the business models "resource recovery" this study presents an opportunity for the valorization of industrial and urban wastes, using alkaline activation technology, to produce hybrid binding materials with a slight amount of cement and lower carbon footprint than conventional Portland-based binders.

Applying the Response Surface statistic methodology, several binding materials were produced based on a mixture of clay brick waste and fly ash in 50/50 proportions with a 10% Portland cement addition. The precursors were activated with an alkaline solution made of sodium silicate and sodium hydroxide. The design factors chosen for the experiment were the molar ratios $SiO_2/Al_2O$ [3.5-4.5] and $Na_2O/SiO_2$ [0.10-0.25], the response variable was the compressive strength of the materials at an age of 28 days.

Based on the experimental data, five mixes with potential use as a cementitious binder were selected as preliminary systems. Different properties and characteristics were evaluated, including compression strength at early ages, carbon footprint, cost and setting time. The microstructure of the selected materials was also evaluated using SEM and FTIR techniques to identify reaction products formation with time.

The hybrid systems reached up to 50 MPa at 28 days of curing. The longest setting time was 234 minutes and the carbon footprints varied from 0.31-0.53 kg-$CO_2$-eq/kg. It was determined that the system made with $SiO_2/Al_2O_3$ and $Na_2O/SiO_2$ of [4.1] and [0.18] respectively, is the most suitable to produce ceramic lightweight composites, as it shows a balance between functional and environmental criteria.

**Keywords:** Circular economy, Alkaline activation, Hybrid binder, Clay brick waste, Fly ash.

## Oral Session 5A: Nanostructured Materials, Sensors

**Time: 08:30-12:25, August 4, 2021.** Eastern European Summer Time
**Session Chair: Dr. Hasan Koten, Istanbul Medeniyet University, Turkey**
***Session Room Link: http://www.academicconf.com/teamslink?confname=cmse2021***

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|---|---|---|
| 08:30-08:55 | **CMSE4523** | Special Applications in the Nanomaterial Technology<br>*Dr. Hasan Koten, Mechanical Engineering Department, Istanbul Medeniyet University, Turkey* |
| 08:55-09:20 | **CMSE4491** | Graphene Based Metal Oxides Nanocomposites and Their Potential Applications<br>*Assoc. Prof. Muhammad Akhyar Farrukh, Department of Chemistry, Forman Christian College (A Chartered University), Pakistan* |
| 09:20-09:35 | **CMSE4488** | Application of Cost Effective Candle Soot in Gas Sensing Technology<br>*Shivani Dhall, Department of Physics, DAV College, India* |
| 09:35-09:50 | **CMSE4561** | Synthesis of Well-ordered Co-Nanoparticles Modified Carbon Nanotubes and Its Application for Highly Sensitive Determination of Phosphate<br>*Ms. Shaimah Rinda Sari, Graduate School of Science and Engineering, Saga University, Japan* |
| 09:50-10:05 | **CMSE4485** | Electrochemical Preparation of Ternary Nonprecious Metal Oxides Nanocomposite and Evaluation of Their Synergistic Effect on Ethanol Oxidation Reaction<br>*Ms. Masoumeh Ghalkhani, Electrochemical Sensors Research Laboratory, Department of Chemistry, Faculty of Science, Shahid Rajaee Teacher Training University, Iran* |
| 10:05-10:30 | **CMSE4524** | $CeO_2$ Nanoparticles Embedded in Different Cellulosic Substrates: Photocatalytic Materials for Pollutant Removal or Organic Reactions<br>*Dr. Andreea-Laura Chibac-Scutaru, Polyaddition and Photochemistry Department, Petru Poni Institute of Macromolecular Chemistry, Romania* |
| 10:30-10:40 | | **BREAK** |
| 10:40-11:05 | **CMSE4525** | Electrical Conductivity of Polymer/Carbon Nanoparticles Composites<br>*Prof. Sergei Bronnikov, Russian Academy of Science, Institute of Macromolecular Compounds, Russia* |
| 11:05-11:20 | **CMSE4496** | Graphene based Nanocomposites and their Supercapacitor Applications<br>*Dr. Aqsa Arshad, Department of Physics, International Islamic University, Pakistan* |
| 11:20-11:45 | **CMSE4493** | Nanocomposite 2D Material Matrix for Battery Anode Materials<br>*Dr. Pratap Kollu, CASEST, School of Physics, University of Hyderabad, India* |
| 11:45-12:00 | **CMSE4571** | Self-assembled Chelating Dithiol on Gold Electrode: Application for Ultra-Sensitive Sensing Copper(II) Ions<br>*Dr. Inderpreet Kaur, Department of Chemistry, Centre for Advanced Studies, Guru Nanak Dev University, India* |
| 12:00-12:25 | **CMSE4463** | Nanocomposites of Polysaccharides with $Ca^{2+}$ and Their Applications in Sensors and Catalytic Conversion of Cr(VI) to Cr(III)<br>*Prof. Farid Khan, Dr. HariSingh Gour Central University, India* |

# Abstracts of Session 5A

**CMSE4523**
**Special Applications in the Nanomaterial Technology**

Hasan Koten
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**Abstract.** In this study different nanostructures have been synthesized and deposited on p-type porous silicone to investigate their photovoltaic properties. The morphology of the synthesized structures has been investigated via scanning electron microscopy and it has been determined that the structures are in the nanoscale. Energy dispersive spectroscopy has been used to investigate the composition of the synthesized structures, and it has been determined that they have defects. The absorption measurements have been performed by ultraviolet-visible spectrophotometry. Based on these absorption measurements, the band gaps of the nanostructures have been calculated as 3.11 eV for spherical ZnO, 3.12 eV for flowers ZnO and 3.64 eV for ZnS. The nanostructures were deposited to obtain thin films in different thicknesses by using a spin-coating method on porous p-type silicone substrates, and then the photovoltaic and electrical properties were investigated. According to the obtained experimental results, it has been determined that the photovoltaic properties of the sample depend on the film thickness. Consequently, ZnS and n-type ZnO nanostructures have been synthesized by a sol-gel method and it has been found that they have photovoltaic properties.

**CMSE4491**
**Graphene Based Metal Oxides Nanocomposites and Their Potential Applications**

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**Abstract.** Green, Bio and Chemical methods have been used to synthesize the nanocomposites containing rare earth-transition metal oxides for the purpose to achieve enhanced activities for their applications in degradations of textiles pollutants, pesticides, organic pollutants, explosive materials etc. Other applications like hydrogenation reactions, slow release fertilizers, forensics, nanofiltration and solar cells have also been studied.

We have successfully synthesized more than 50 nanocompostes with variety of metals. Multiple approaches have been carried out to synthesize the rare earth-transition metal oxides nanocomposites as well as reduced reduced graphene oxide doped with metal oxides nanocomposites. Various factors e.g. change in precursors, pH, temperature, feed rate, surfactants, solvents, methods of preparation, concentration of precursors, were studied which change the efficiency of the nanocomposites. Our focus is to synthesize nanocomposites having band gap in the visible region so that they may be used for enhanced catalytic activity under sun light.

The influence of surfactants and solvents on the activities of nanocomposites for their application in waste water treatment in chemical industries was studied and nanofiltration system was developed.

The structural investigation, thermal degradation, crystallite size, morphology, surface and photocatalytic properties of synthesized samples were studied by using different characterization techniques i.e. Thermogravimetric analysis (TGA), *Differential scanning calorimetry* (*DSC*) Fourier transform-infrared spectroscopy (FTIR), Particle Size Analyzer (PSA), Powder X-ray diffraction (XRD), Scanning electron microscopy (SEM), Transmission electron microscopy (TEM), and Ultraviolet-Visible spectrophotometer (UV-VIS).

**CMSE4488**

**Application of Cost Effective Candle Soot in Gas Sensing Technology**

Shivani Dhall

*Department of Physics, DAV College, Jalandhar, Punjab, India*

**Abstract.** In recent years, carbon materials are widely investigated because of they are enormously sensitive to hydrogen ($H_2$) at room temperature conditions. In the present work, the inexpensive candle carbon soot (CCS) is used to detect 0.5% concentration of $H_2$ gas at room temperature. A simple flame of candle is used to synthesize the layers of carbon soot at room temperature conditions. It is observed that, the acid treatment of CCS drastically improved their structural and sensing properties as compared to as-synthesized CCS. The effect of acid functionalization on the CCS structure were investigated by X-ray diffraction (XRD) and Raman spectroscopy. To the best of our knowledge, detection of low concentrations of $H_2$ gas is reported here for the first time using economical CCS at room temperature. These results are important for developing a new class of chemiresistive type gas sensor based on change in the electronic properties of the CCS.

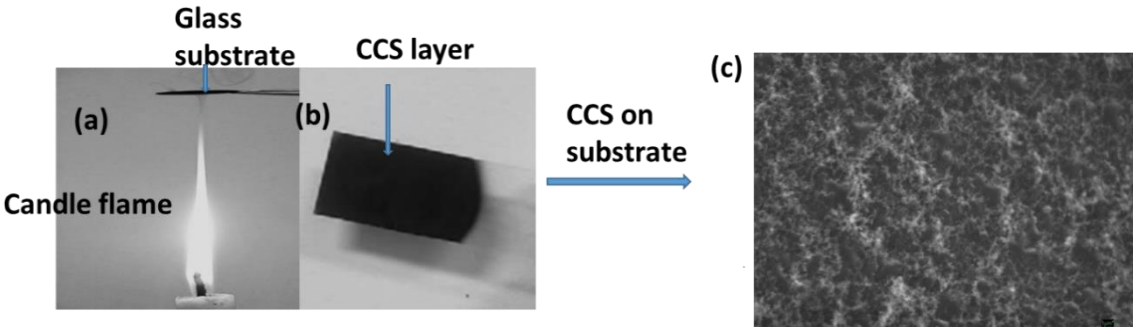


Figure. Synthesis of CCS film (a) a glass substrate is held in the flame of a candle (b) a thick CCS layer (c) SEM image of CCS layer.

**CMSE4561**

# Synthesis of Well-ordered Co-Nanoparticles Modified Carbon Nanotubes and Its Application for Highly Sensitive Determination of Phosphate

Shaimah Rinda Sari[1], Masayuki Tsushida[2], Tetsuya Sato[2] and Masato Tominaga[1,*]
[1]*Graduate School of Science and Engineering, Saga University, Japan*
[2]*Faculty of Engineering, Kumamoto University, Japan*

**Abstract.** Phosphorus is one of essential nutrients for plant which usually supplied to the crops via fertilizer. However, excess amount of fertilizer might cause leaching of phosphate from agricultural land leading to eutrophication. Consequently, sensors capable of detecting phosphate ions at concentrations below the eutrophication threshold (0.1 μM) are highly desirable. In recent decades, considerable attention has been directed toward the development of electrochemical phosphate sensors in view of their simple operation, fast response, and high sensitivity. Cobalt electrode especially cobalt-based nanomaterials has been known to be used for phosphate ion detection owing to their large specific surface areas, excellent conductivities, catalytic activities and their ability in sensing phosphate ion. In this study, the cobalt nanoparticles (CoNPs) modified electrode was synthesized together with polybenzimidazole (PBI) and multi-walled carbon nanotube (MWCNT) for the determination of phosphate ion with high sensitivity (Fig. 1). Synthesized CoNPs featured unique square shape and a uniform size (3.5–5.5 nm), mainly containing hexagonal $Co_3O_4$. The effect of morphology and microstructures on the electrochemical performance was investigated and the CoNPs modified electrode exhibited better phosphate sensing performance than previously reported polycrystalline Co wires. Specifically, the electrode also could sense phosphate at pH 7 at a range concentration of 0.1–100 nM (Fig. 2), which is lower than the eutrophication threshold and also lower than the ability of previously reported Co wire electrode (i.e. 10 μM–0.1 M). The electrode was successfully used to detect phosphate in actual creek water samples. All these remarkable performances suggest that the proposed CoNPs/PBI/MWCNT/GCE is a promising candidate for phosphate ion detection.

**Keywords:** Electrochemical sensor, Phosphate ion, Cobalt, Metal nanoparticles

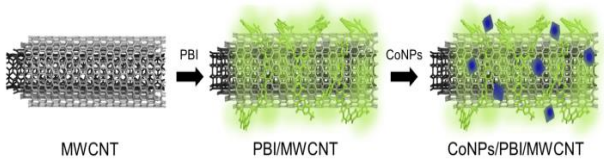


Figure 1. Schematic of the CoNP/PBI/MWCNT composite.

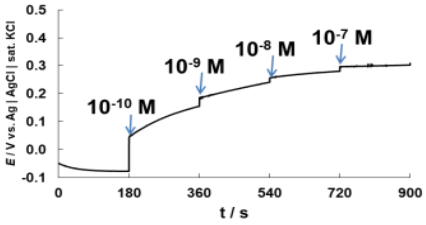


Figure 2. Open-circuit potentials (E) obtained for CoNPs/PBI/MWCNTs/GCE at different phosphate concentrations at pH 7.

**CMSE4485**

## Electrochemical Preparation of Ternary Nonprecious Metal Oxides Nanocomposite and Evaluation of Their Synergistic Effect on Ethanol Oxidation Reaction

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[2]*Fuel Cell Research Laboratory, Faculty of Science, Shahid Rajaee Teacher Training University, Lavizan, P.O. Box 1678815811, Tehran, Iran*

**Abstract.** The GCE surface was modified by electrodeposition of a combination of oxides of nonprecious metals, Cu, Ni and Fe. The modification process was performed through one step electrodeposition or layer by layer steps. The metallic Ni was electrodeposited from a Watts bath solution containing $Fe_2O_3$ nanoparticles that co-deposited on the GCE surface with Ni ions. Prepared electrodes by two consecutive steps of electro-deposition were named as Ni,$Fe_2O_3$/Cu/GCE and Cu/Ni,$Fe_2O_3$/GCE, for which first the Ni,$Fe_2O_3$ layer and then Cu layer were deposited or vice versa, respectively. In one step procedure, the all components were simultaneously electrodeposited on the GCE, which defined as Cu,Ni,$Fe_2O_3$/GCE. The GCEs modified with metal oxide nanostructures were activated by CV cycling in alkaline solution and their electro-catalytic activity was tested toward ethanol electro-oxidation reaction (EOR). The physicochemical and electro-catalytic characterizations of the fabricated electro-catalysts were evaluated by scanning electron microscopy, elemental mapping analysis, voltammetry and chronoamperometry. The best performance regarding decreasing the EOR overpotential and enhancing its oxidation current was observed for Cu,Ni,$Fe_2O_3$/GCE. The fast and facile engineered design of the GCE modification with the ternary Cu,Ni,$Fe_2O_3$ components led to achievement of high current density of about 101 mA/cm$^2$ with high reduced tolerance against poisoning intermediates and therefore longtime stability for the EOR in alkaline media. The synergistic effect between Ni, Cu and Fe oxides nano-particles provided promising properties for EOR pursuing construction of the powerful devise with commercialization potential.

**Keywords:** Copper oxide, Nickel oxide, Ethanol, Electrochemical, Oxidation.

**CMSE4524**

## $CeO_2$ Nanoparticles Embedded in Different Cellulosic Substrates: Photocatalytic Materials for Pollutant Removal or Organic Reactions

Andreea-Laura Chibac-Scutaru[*], Violeta Melinte
*Polyaddition and Photochemistry Department, Petru Poni Institute of Macromolecular Chemistry, Romania*

**Abstract.** Photocatalysis plays a pivotal role in today's global issues, meeting the requirements of sustainable chemistry and green organic synthesis, with applications in a large variety of processes, from organic pollutants mineralization to fine organic reactions. $CeO_2$ NPs is a feasible „platform" for the next generation of photocatalysts, since $CeO_2$ has a band gap similar to $TiO_2$ NPs (Eg = 3.19 eV), a particular outer electron configuration (*[Xe] 4f$^1$5d$^1$6s$^2$*) that enhance the electron transfer, low price (6.36 USD/kg in 2018), reversible shift of the oxidation state between $Ce^{3+}$ and $Ce^{4+}$, in the cubic

fluorite structure form oxygen vacancies, are long-term stable and nontoxic. Unfortunately, the use of inorganic nanoparticles as photocatalysts is limited by their agglomeration tendency, which leads to a decrease in their surface area and eventually of their photocatalytic efficiency, but also to the difficulties encountered during their separation and reuse. To overcome these drawbacks, in the literature was emphasized that the use of various polymers as supports for the efficient immobilization of active photocatalytic nanoparticles could represent a viable solution, due to some unquestionable advantages of polymeric supports: resistance to ultraviolet radiations, high durability, chemical stability, and easy availability.

In view of all these information, this study reports the design of multiple cellulose-derived platforms for efficient immobilization of pristine/functionalized $CeO_2$ nanoparticles. The resulted nanocomposites were successfully tested as photocatalysts for the photodegradation under UV irradiation of the hazardous pollutants methyl orange, Congo red and 4–nitrophenol or for the photoreduction reaction of 4–nitrophenol. The reusability of the photocatalysts after several cycles and their efficiencies under visible irradiation were also tested.

**Keywords:** $CeO_2$ NPs, Surface nanoparticles functionalization, Cellulosic matrix, Cellulose regeneration/oxidation, Photocatalysis/photoreduction.

**Acknowledgements:** This work was supported by a grant of the Romanian Ministry of Education and Research, CNCS–UEFISCDI, project number PN-III-P1-1.1-TE-2019-1245 (23/27.08.2020), within PNCDI III.

**CMSE4525 To avoid repeatability issues, this abstract will be available after the full paper is published in the conference proceedings.**

**CMSE4496**
**Graphene based Nanocomposites and their Supercapacitor Applications**

Aqsa Arshad
*Department of Physics, International Islamic University, Pakistan*

**Abstract.** A great many products including portable and wearable electronic devices, electrical vehicles have reached the frontier of current clean energy technology research. There have been observed great improvements in different aspects of these technology-based devices over past few years, however, the energy storage i.e., batteries that are the key power source of electronics, significantly lagged the development of portable electronics. Owing to unending demands of users, it is desirable to use supercapacitors. In this work, a series of ferrite/GNPs nanocomposites ($CoFe_2O_4$/GNPs, Zn $Fe_2O_4$/GNPs, Mg $Fe_2O_4$/GNPs, Ca $Fe_2O_4$/GNPs and Cu $Fe_2O_4$/GNPs) were fabricated using a wet chemical route. The synthesized nanocomposites were characterized for their crystalline phase, morphology, chemical state, band gap, vibrational modes, and photoluminescence. The composites were further evaluated for their performance as supercapacitor materials. A highest specific capacitance and energy density has been observed for Mg $Fe_2O_4$/GNPs (50%) nanocomposites.

**CMSE4493**

**Nanocomposite 2D Material Matrix for Battery Anode Materials**

Pratap Kollu*

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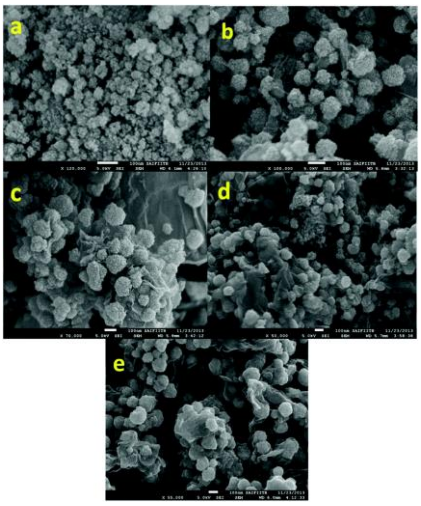
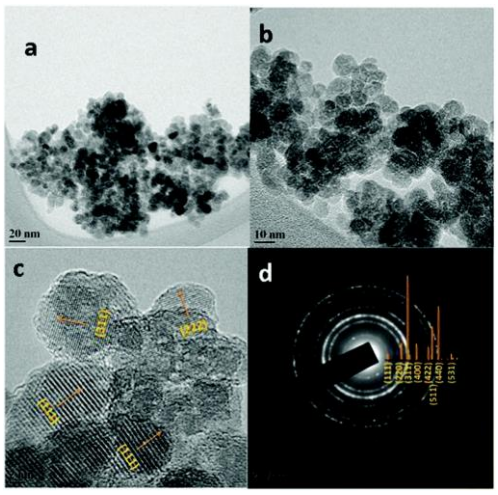
**Abstract.** Porous $CoFe_2O_4$ nanoclusters with different concentrations of graphene based composites were synthesized by a simple solvothermal process. The electrochemical properties of prepared $CoFe_2O_4$–reduced graphene oxide (rGO) composites were evaluated using polyvinylidene fluoride and Na-alginate as binder materials.

The synthesized porous $CoFe_2O_4$–rGO composites were characterized using an X-ray diffractometer (XRD, X'pert PRO MPD, PANalytical, Philips) with Cu Kα radiation ($\lambda$ = 1.54 Å at 40 kV and 30 mA). The size and shape of synthesized samples were examined using Field Emission Scanning Electron Microscopy (FESEM)-EDS (JSM-7600F, JEOL). Transmission electron microscopy with energy dispersive spectroscopy (TEM), JEOL 2010F HRTEM, Japan, with 200 kV operating voltage was used to capture the morphology and crystallinity of porous $CoFe_2O_4$–rGO composite samples. The $CoFe_2O_4$ + 20% rGO composites with alginate binders deliver a stable maximum discharge capacity of 1040 mA h $g^{-1}$ at 0.1 C, which is nearer to the theoretical capacity (914 mA h $g^{-1}$) of this material. The alginate binders hold the integrity of the electrode and 20% rGO will give the electron transportation network during the conversion reaction in $CoFe_2O_4$ + 20% rGO composites/alginate electrodes.




FESEM images for the (a) pure CoFe2O4, (b) CoFe2O4 + 10% rGO, (c) CoFe2O4 + 20% rGO, (d) CoFe2O4 + 30% rGO, (e) CoFe2O4 + 40% rGO composites.




HRTEM images at different magnifications, (c) high resolution images and (d) SAED ring patterns for the pure porous CoFe2O4 nanoclusters.

**CMSE4571**

**Self-assembled Chelating Dithiol on Gold Electrode: Application for Ultra-Sensitive Sensing Copper(II) Ions**

Inderpreet Kaur

*Department of Chemistry, Centre for Advanced Studies, Guru Nanak Dev University, Amritsar, Punjab - 143005, India*

**Abstract.** Copper is a third most abundant heavy metal on the earth (after $Fe^{2+}$ and $Zn^{2+}$) and occur in water (rivers, oceans & lakes), rocks and earth crust at low level. It is mainly present in many food sources such as seafood, organ meats, grain products etc. Humans are exposed to copper via contaminated drinking water/food and other environmental sources which pose an increasing threat to healthy functioning of life-sustaining metabolic activities and demands regular monitoring of copper content in the environment, i.e. soil and water. In the present work, chelating dithiol, bis(3-((5-mercapto-1,3,4-thiadiazol-2-yl)carbamoyl)phenyl)terephthalate (BMTCPT) was synthesized and self-assembled on the surface of gold electrode which allows the formation of macrocycle capable of accommodating metal ions. Self-assembly of dithiol was confirmed by electrochemical techniques: cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) in two redox probes: anionic, $[Fe(CN)_6]^{3-/4-}$ and cationic, $[Ru(NH_3)_6]^{2+/3+}$ and further, utilized as a platform for impedimetric sensing for $Cu^{2+}$. EIS studies showed that Au-BMTCPT electrode displayed a very sensitive and selective response towards $Cu^{2+}$ in wider linear concentration range from $1\times10^{-12}$ M to $1\times10^{-5}$ M ($r^2$ = 0.990) at pH = 5 with lower detection limit of $9.7x10^{-13}$ M. In addition, dithiol self-assembled gold nanoparticles (BMTCPT-AuNPs) were applied to construct a chemically modified carbon paste electrode (CPE) and subjected to potentiometric detection of $Cu^{2+}$ which exhibited a Nernstian slope of 29.85±0.2 mV per decade in concentration range of $1\times10^{-9}$ M - $1\times10^{-4}$ M ($r^2$ = 0.999) with a detection limit of $8.91\times10^{-10}$ M.

**Keywords**: Chelating dithiol, Cyclic voltammetry, Electrochemical impedance spectroscopy, Self-assembly, Copper (II) ions, Carbon paste electrode.

**Acknowledgements:** The financial support from the Science & Engineering Research Board, Department of Science and Technology (SERB- DST), New Delhi is acknowledged.

**CMSE4463**

**Nanocomposites of Polysaccharides with $Ca^{2+}$ and their Applications in Sensors and Catalytic Conversion of Cr(VI) to Cr(III)**

Farid Khan

*Nanomaterials Discovery Laboratory, Department of Chemistry, Dr. HariSingh Gour Central University, SAGAR-India*

**Abstract.** Polysaccharides are a diverse class of polymeric materials of natural (animal, plant, algal) origin formed via glycosidic linkages of monosaccharides and are known for making composites when they are crosslinked with di or tri valent cations. Such materials are non-toxic, economically viable, easily available and environmentally benign. The applications are many like sensors, targeted drug delivery, tissue engineering, catalytic conversion of toxic metals and bound heeling. Worldwide, industrial development increases the toxic metals such as As, Hg, Cd and Cr in soil and ground water. Amongst these metals, Cr(VI) is emerged as the most hazardous metal to living things. The excess amount of Cr(VI) generated by electroplating, leather tanning, metal policing, pigment industry, cooling tower, steel manufacturing and photography causes severe problem in kidney, liver, vomiting, diarrhea and skin disorder. Several methods are available for the removal of Cr(VI) including adsorption, bio-sorption, electro coagulation, ion exchange, filtration and photo catalytic reduction. Herein, electrochemical method is used to determine Cr(VI) using Alginate(alg.) /Carboxymethylcellulose(CMC)/Dextran(Dex.)/$MnO_2$/g-$C_3N_4$/Ca with detection limit of 0.63 ng/mL which is the lowest limit reported so far. The UV-Vis. spectroscopy is used to reduce Cr(VI) to Cr(III) in presence of $NaBH_4$ just in 26.63 s without using $H_2SO_4$ which is toxic and the reaction kinetic become uncontrolled when $H_2SO_4$ is used.

## Oral Session 5B: Nanostructured Materials, Sensors

**Time: 14:15-18:05, August 4, 2021.** Eastern European Summer Time

**Session Chair: Assoc. Prof. Jun Yan, University of Massachusetts Amherst, USA**

***Session Room Link: http://www.academicconf.com/teamslink?confname=cmse2021***

| | | |
|---|---|---|
| 14:15-14:30 | **CMSE4591** | Microwave Digested Rapid Method for Extraction $SiO_2$ Nano Particles from Agricultural Waste - Wheat Straw<br>*Dr. Khushbu Patel, School of Science, Rai University, India* |
| 14:30-14:45 | **CMSE4601** | Effect of Adding CeO Nano Particles onto Magnetic Carbon Nano Tube to Preconcentrate Acid Brown-14<br>*Dr. Parastoo Jamshidi, School of Chemistry, College of Science, University of Tehran, Iran* |
| 14:45-15:10 | **CMSE4513** | Electronically Induced Emission of Methane Decomposition Products – Excited Hydrogen Atom Desorption from Ar Cryomatrices<br>*Dr. Elena Savchenko, B. Verkin Institute for Low Temperature Physics & Engineering NASU, Ukraine* |
| 15:10-15:25 | **CMSE4518** | The Influence of Annealing Process on the Properties of $TiO_2$ and NiO Metal Oxide Thin Films<br>*Dr. Ivan Košč, Department of European Integrated Management of Borders, Academy of the Police Force in Bratislava, Slovakia* |
| 15:25-15:40 | **CMSE4527** | Recent Progress and Perspectives of Gas Sensors Based on Nanomaterials<br>*Dr. Daniel Matatagui, Instituto de Tecnologías Físicas y de la Información (ITEFI), CSIC, Spain* |
| 15:40-15:55 | **CMSE4497** | Self-Organization of Silver Nanoparticles in a $TiO_2$ Matrix for Plasmonic Applications: Analytical Modeling and Kinetic Monte Carlo Simulations<br>*Dr. Adil Bouhadiche, Research Unit in Optics and Photonics (UROP), Center for Development of Advanced Technologies (CDTA), University of Setif 1, Algeria* |
| 15:55-16:20 | **CMSE4556** | Self-assembly of Semiconductor Quantum Dots with Porphyrin Molecules: Surface Morphology, Energy Relaxation Pathways and Exciton-Phonon Coupling<br>*Dr. Eduard Zenkevich, Belarussian National Technical University, Minsk, Belarus* |
| 16:20-16:30 | | **BREAK** |
| 16:30-16:55 | **CMSE4505** | Sustainable Porous Material Derived from Industrial By-Products for Airborne Particulate Matter Entrapment<br>*Dr. Alessandra Zanoletti, INSTM and Chemistry for Technologies Laboratory, Department of Mechanical and Industrial Engineering, University of Brescia, Italy* |
| 16:55-17:20 | **CMSE4568** | Improving Exciton Valley Polarization by Scattering<br>*Assoc. Prof. Jun Yan, Department of Physics, University of Massachusetts Amherst, USA* |
| 17:20-17:35 | **CMSE4583** | Graphene Oxide Magnetic Nanocomposites for Degradation of Dye Congo Red from Wastewater<br>*Dr. Azam Zamani, Department of Chemistry, Science and Research Branch, Islamic Azad University, Tehran, Iran* |

| | | |
|---|---|---|
| 17:35-17:50 | **CMSE4584** | Synthesis, Characterization and Photoelectrochemical Properties of $ZnO/Fe_2O_3$, ZnO/MOF and ZnO/Biosilica Composited Films<br>*Mr. Gabriel Yuji Hata, Institute of Marine Sciences, UNIFESP, Brazil* |
| 17:50-18:05 | **CMSE4614** | Preparation and Characterization of Nanocellulose and its Application<br>*Dr. T.H.S. Flores-Sahagun, Federal University of Parana (UFPR), Brazil* |

# Abstracts of Session 5B

**CMSE4591**

**Microwave Digested Rapid Method for Extraction $SiO_2$ Nano Particles from Agricultural Waste - Wheat Straw**

Khushbu Patel
*School of Science, Rai University, Ahmedabad, Gujarat, India*

**Abstract.** Substantial applications of silica materials in industrial products have caused development of silica extraction methodologies out of various waste products. Agricultural wastes including rice husk/straw and wheat husk/straw are one of the coast effective sources which have a huge content of silicate materials. Microwave assisted process was found to be cost effective, rapid, easy and an economically viable method compared to other methods. Microwave-assisted acid digestion, followed by calcination of the charred product of wheat straw are resulted in 100-200 nm-sized amorphous silica (WS-n$SiO_2$) with specific surface area in high yields without generating considerable smoke and airborne particulates. The nano $SiO_2$ extracted from wheat straw was characterized by fourier-transform infrared (FTIR) spectroscopy, X-ray diffraction (XRD) analysis, particle size analysis, energy-dispersive X-ray (EDX) analysis, and scanning electron microscopy (SEM). This analytical study shows that the produced silica is nano sized, amorphous, meso-pouros silica. This methodology can be used in future for production of pure, nano sized and high amount of silica from agricultural waste.

**Keywords:** Nano Silica, Wheat straw, Microwave digestion, Calcination.

**Acknowledgements**. Author is grateful to Dr. Manoj Pandey, Assoc. Professor from 'Pandit Deendayal Petroleum University' for help in acquiring analytical facilities.

**CMSE4601**

**Effect of Adding CeO Nano Particles onto Magnetic Carbon Nano Tube to Preconcentrate Acid Brown-14**

Parastoo Jamshidi
*School of Chemistry, College of Science, University of Tehran, PO. Box 14155-6455, Tehran, Iran*

**Abstract.** The pollutants released into the environment cause negative effects and consequences on the human body, plants and animals. Hence, researchers have proposed a number of preconcentration methods, one of which is magnetic solid phase extraction. In this method, a magnetic adsorbent extracts the target analyte followed by being eluted via appropriate eluent. A nanocomposite of carbon nano tube-$Fe_3O_4$ (mCNT) is highly applicable to preconcentrate azo dyes, because of π-π interaction between carbonic components and dyes. However, modification by oxides of lanthanide series could increase the positive charge of adsorbents because of charge transfer to their empty orbitals, which enhances the electrostatic forces between analyte and adsorbents and raises the preconcentration efficiency. Accordingly, mCNT was prepared and then dispersed in a solution of Ce(NO3)3.6H2O,

finally cerium oxide was structured in the presence of NH3. Box–Behnken design was applied to find the optimum conditions of acid brown -14 (AB-14) preconcentration, prior to its quantification by UV–Vis spectrophotometer ($\lambda$ = 480 nm). It decreases the usage amount of adsorbent and minimizes the preconcentration time. The optimum condition is as follows: pH of 5 ± 0.2, adsorbent dose of 10 mg, adsorption time of 20 minutes, eluent of DMF and desorption time of one minute. Reusability, durability, limit of detection, relative standard deviation, preconcentration factor and linearity of dynamic range confirm performance of the adsorbent. Swelling behavior, isotherm of adsorption, kinetic of adsorption and thermodynamic of adsorption were investigated. Real samples of wool and silk were successfully applied to preconcentrate AB -14.

**Keywords:** CeO, Carbon nanotube, Acid Brown 14, Preconcentration, Magnetic solid phase extraction.

**CMSE4513**

## Electronically Induced Emission of Methane Decomposition Products – Excited Hydrogen Atom Desorption from Ar Cryomatrices

E.V. Savchenko*, I.V. Khyzhniy, M.A. Bludov, S.A. Uyutnov
*B. Verkin Institute for Low Temperature Physics & Engineering NASU, Ukraine*

**Abstract.** Radiation effects in solids attract much attention in diverse fields such as material and surface sciences, particle physics, physics and chemistry of interstellar and solar systems. Emission of particles or desorption is among the most intensively studied radiation-induced phenomena. This phenomenon is of fundamental importance by itself, moreover, it provides essential information on radiation-induced processes in solids. The most part of studies on radiation-induced particle emission are carried out using mass-spectroscopy methods. Such an approach presents a way to obtain data on element composition of desorbing particles, their velocities, but not on their electronic states. We applied luminescence spectroscopy method to elucidate states of hydrogen atom desorbing from $CH_4$-doped Ar matrix exposed to an electron beam. The essential feature of $CH_4$ molecule is an absence of any radiative transitions from the molecule itself. An excitation of $CH_4$ results in its dissociation with an appearance of different fragments (H, $CH_3$, $CH_2$, CH and $H_2$) and H fragment appeares in most reactions. In this study we focused on the desorption of H atoms at subcritical dose of irradiation with an electron beam. The measurements were carried out in the range of a $CH_4$ concentration from 0.1 % to 10 %. A prepared CH4/Ar gas mixture was condensed on a Cu substrate at LHe temperature. Irradiation was performed in a dc mode with 1.5 keV electron beam. Luminescence spectra were recorded in the VUV and visible ranges. Cathodoluminescence (CL) spectra of $CH_4$-doped Ar matrices contain emission bands of the matrix as well as CL bands of $CH_4$ dissociation products: bulk emissions of CH, C, $Ar_2H^*$ and emission of desorbing $H^*$ atoms – the Ly – α line. Two scenario of $H^*$ atom production are suggested which involve holes and excitons of the matrix. In view of high ionization potential of the matrix exceeding those of the dissociation products efficient charge transfer occurs with $CH_4^+$ production. Deprotonation to the matrix results in $H^+$ formation followed by its radiative recombination with electron and generation of excited $H^*$ atoms emitting the Ly – α line ($H^+ + e \rightarrow H^{**} \rightarrow H^* \rightarrow h\nu$). The second likely route involves excitons. Transfer of energy from the exciton $\Gamma$ 3/2 n=1 results in a direct population of the n=3 level of H atom followed by its relaxation to the n=2 level and the Ly – α emission. Concentration behavior of the phenomenon and its connection with other processes in the bulk are discussed.

**Keywords:** Methane, Matrix isolation, Hydrogen, Electron irradiation, Luminescence, Desorption.

**CMSE4518**

**The Influence of Annealing Process on the Properties of $TiO_2$ and NiO Metal Oxide Thin Films**

Ivan Košč

*Department of European Integrated Management of Borders, Academy of the Police Force in Bratislava, Slovakia*

**Abstract.** The influence of annealing process on the compositional, structural, morphological, optical, and electrical properties of single and compound $TiO_2$ and NiO metal oxide thin (nanoscale) films. The examined thin films were prepared by dc magnetron sputtering technique. The scanning electron microscopy (SEM) observation of the prepared samples confirm presence of thin films on the top of the deposition substrate. The structural parameters have been investigated by X-ray diffraction (XRD). The identified diffraction patterns revealed strong influence of thermal annealing process on the crystallinity of the $TiO_2$/NiO thin films. The structural parameters are generally influenced by the deposition technique parameters. In the range of tested annealing temperatures, the crystallization started, and the structure of the thin films changed from amorphous to polycrystalline. The morphology of the as-deposited and annealed samples has been investigated by atomic force microscopy (AFM). Roughness of the surface was identified (in consideration of the dc magnetron sputtering method) and compared according to the parameter of annealing temperature. The optical parameters of the thin films have been investigated by the optical transmittance measurements. The presence of the differences in the position of leading edge of the transmittance spectra of as-deposited and annealed samples identified strong influence of annealing process (also deposition parameters) on the properties of the metal oxide $TiO_2$ and NiO thin films. Acknowledgements: This work was supported by the Slovak University of Technology in Bratislava, Faculty of Electrical Engineering and Information Technology, Institute of Electronics and Photonics and by the Academy of the Police Force in Bratislava (Slovakia).

**Keywords:** Thin films, Metal oxides, TiO2, NiO, Annealing, Magnetron sputtering.

**CMSE4527**

## Recent Progress and Perspectives of Gas Sensors Based on Nanomaterials

Daniel Matatagui* and María del Carmen Horrillo
*Instituto de Tecnologías Físicas y de la Información (ITEFI), CSIC, Serrano 144, 28006 Madrid, Spain*

**Abstract.** In recent decades has occurred a growing investigation about solid-state sensors in order to develop technologies for detecting toxic gases and biomarkers. However, it is only now that these miniaturized and low cost devices, combined with nanotechnology are becoming promising candidates for monitoring air quality, detecting and identifying hazardous compounds to human health. In this work, graphene-based materials, metal oxide nanoparticles, nanowires, nanotubes and graphene have been under study. These nanostructured materials have been incorporated as new sensitive layers on devices based on surface acoustic wave, spin waves and resistive platforms. The results obtained so far have shown these nanostructured materials provide new advantages, such as, a dramatic increase in sensitivity, high selectivity, faster response of the sensor, and low power consumption. The above sensors have been developed and characterized in different toxic environments, proving their high efficiency, leading to real-time detection and detecting parts per trillion of some toxic compounds.

**Keywords:** Nanomaterial, Gas sensor, Toxic gases, 2D marterials, Biomedical applications.

**Acknowledgements:** The authors acknowledge the Spanish Ministry of Science and Innovation for financing the project RTI2018-095856-B-C22 (AEI/FEDER). Daniel Matatagui acknowledges the financial support from the Fundación General CSIC via Programa ComFuturo.

**CMSE4497**

## Self-Organization of Silver Nanoparticles in a $TiO_2$ Matrix for Plasmonic Applications: Analytical Modeling and Kinetic Monte Carlo Simulations

Adil Bouhadiche[1,*], Soulef Benghorieb[1] and Tahar Touam[2]
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**Abstract.** Due to their peculiar qualities, ordered silver nanoparticles (AgNPs) have been widely used in various fields such as medicine, food, health care, consumer and industrial uses, among others. These include optical, electrical, thermal as well as biological properties. Interestingly, the properties of AgNPs show great sensitivity to the shape and size of NPs, to their local environment as well as to the polarization nature of the incident light and to the coupling between nearby plasmon resonances. In fact, the control of the surface morphology and hence the physical properties of light-ordered plasmonic silver nanostructures has been successfully studied in titanium dioxide ($TiO_2$) films since $TiO_2$ has become the best candidate, among TCO materials, due to its promising properties in several applications. This article aims, via the kinetic Monte Carlo (KMC) method, to investigate the process of self-organized growth of AgNPs in a thin film of amorphous $TiO_2$ under excitation of light. First, the deposition phase of $TiO_2$ thin films obtained by a sol-gel technique is studied by selecting the deposition rate as the most influential main parameter. Next, a new simulation model describing the

spontaneous formation of periodic arrays of smaller spherical AgNPs in a $TiO_2$ matrix is proposed. The origin of the transmission spectra is analyzed over a wider range of wavelengths from 0 to 1000 nm, thanks to the nature of polarization, the angle of incidence and the excitation wavelength.

**Keywords:** $TiO_2$ material, Sol-gel, AgNPs, Self-organization, KMC, Plasmonic applications.

**CMSE4556**

## Self-assembly of Semiconductor Quantum Dots with Porphyrin Molecules: Surface Morphology, Energy Relaxation Pathways and Exciton-Phonon Coupling

Eduard Zenkevich[1,*], Thomas Blaudeck[2], Christian von Borczyskowski[3] and Dietrich R.T. Zahn[3]
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**Abstract.** A "bottom-up" strategy was used for the driven formation of heterogeneous nanoassemblies based on colloidal semiconductor TOPO-capped core/shell CdSe/ZnS quantum dots (QDs) and tetra-pyridylporphyrins (via coordination interactions). Using a quantitative experimental analysis of the QD photoluminescence quenching in QD-porphyrin nanoassemblies as well as theoretical calculations it is shown that the attachment of porphyrin molecules to QD leads to the realization of several competing non-radiative photophysical phenomena: i) non-radiative energy transfer QD→porphyrin of Foerster type; ii) non-FRET processes including electron tunneling beyond the QD core under conditions of quantum confinement; iii) the formation of near band edge states (surface traps). The competition between FRET and non-FRET quenching processes drastically depends on the QD size as well as the solvent polarity and the spatial displacement of porphyrin macrocycles on the QD surface. Based on absorption and photoluminescence data in a temperature range 77-293 K in methylcyclohexane-toluene mixture 6:1 (glassy matrix), the role of the exciton-phonon coupling in nanoassemblies was analyzed taking into account the low-temperature conformational transformation of the surface ligand layer. It was argued that the formation of the absorption band for the first exciton transition in QD takes place with participation of CdSe core LO phonons, while photoluminescence properties reflect also additional interactions with ZnS shell LO phonons. It means, that evaluation of exciton-phonon coupling from Stokes shifts will generally result in too large values.

**Keywords:** semiconductor quantum dots, porphyrins, energy transfer, electron tunnelling, exciton-phonon coupling

**Acknowledgements:** This work was funded by Volkswagen Foundation (Project "New Functionalities of Semiconductor Nanocrystals by Controllable Coupling to Molecules"), BSPSR program "Photonics and Electronics for Innovations (2021-2025)", as well as by the European Union (Grant 732482, Bio4Comp - Parallel Network-Based Biocomputation) in the framework of a Training Period (E.Z.), and Visiting Scholar Program of TU Chemnitz, Germany (E.Z., 2020-2021).

**CMSE4505**

## Sustainable Porous Material Derived from Industrial By-Products for Airborne Particulate Matter Entrapment

Alessandra Zanoletti*, Antonella Cornelio and Elza Bontempi
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**Abstract.** Airborne particulate matter (PM) is a critical issue for the environment and human health. The European Environment Agency (EEA) estimated that $PM_{2.5}$ concentrations in 2018 were responsible for about 379 000 premature deaths originating from long-term exposure in Europe. Nowadays, filters represent the conventional methods widely adopted for PM entrapment. However, the existing materials for air filters are generally petroleum-based materials, with high costs both from an economical and environmental point of view. This work presents innovative porous material (named SUNSPACE "SUstaiNable materials Synthesized from by-Products and Alginates for Clean air and better Environments") which is an affordable and sustainable solution for PM capture. SUNSPACE is realized by using industrial by-products, like silica fume and bottom ash, low-cost materials, and low temperature thermal process. It is characterized by ink-bottle shaped pores, suitable for ultrafine PM entrapment. Different tests were performed to evaluate the ability of SUNSPACE to capture PM in not controlled (such as particles generated by diesel, incense and cigarettes smokes and generated at industry of steel alloy) and controlled conditions (using an aerosol nanoparticles generator). The idea is to apply the material as coating on different supports (such as walls, street borders, roofs) to improve the urban air quality.

**Keywords:** Innovative porous materials, PM capture, Air quality, Sustainability, Circular economy.

**CMSE4568**

## Improving Exciton Valley Polarization by Scattering

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**Abstract.** The advent of atomically thin 2D materials, such as graphene and transition metal dichalcogenide (TMD) semiconductors, has boosted the development of valleytronics. In particular, excitonic valley degree of freedom in TMDs such as monolayer $MoS_2$ can be effectively addressed by optical means. Here we experimentally show a counter-intuitive improvement of valley polarization in $MoS_2$ induced by scattering. We report seven- and twelve-folds of valley polarization enhancement due to thermally activated and charge doping induced scattering respectively. This interesting effect is attributed to the reduction of valley pseudospin precession arising from rapid modulation of exciton momentum and concomitant exchange interaction field, which is analogous to motional narrowing in nuclear magnetic resonance spectroscopy. Our work advances understanding of valley depolarization mechanisms in TMD atomic layers and illustrates a novel approach for controlling and improving valleytronic devices.

**Keywords:** 2D materials, Transition metal dichalcogenide, Valley polarization, Exchange interaction.

**Acknowledgements:** This work is supported by National Science Foundation (NSF, Grant number: DMR-2004474).

**CMSE4583**

## Graphene Oxide Magnetic Nanocomposites for Degradation of Dye Congo Red from Wastewater

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**Abstract.** Magnetic $ZnFe_2O_4$@MnO –graphene oxide and $ZnFe_2O_4$@MnO –reduced graphene oxide nanocomposites were prepared via a facile co-precipitation and hydrothermal methods and characterized by X-ray powder diffraction (XRD), diffuse reflectance UV-vis spectroscopy (DRS), photoluminescence (PL) spectra,Transmission electron microscopy (TEM), field emission scanning electron microscopy (FESEM), Fourier transform infrared spectroscopy (FTIR), vibrating sample magnetometry (VSM) techniques and Bruner-Emmett-Teller (BET). The $ZnFe_2O_4$@MnO, $ZnFe_2O_4$@MnO-GO and $ZnFe_2O_4$@MnO-rGO nanoparticles were found to have a size of 20-40 nm and were spread out on the graphene oxide nanosheets and reduced graphene oxide nanosheets. Magnetic studies demonstrated that the $ZnFe_2O_4$@MnO–graphene oxide and $ZnFe_2O_4$@MnO – reduced graphene oxide nanocomposites can be easily separated from the solution by an external magnetic field. The photocatalytic degradation of Congo red dye (CR) was evaluated based on the removal of Congo red (CR) in aqueous solution under visible light irradiation. The photocatalytic activity was affected by the structural and optical properties as well as the surface area of the samples. Compared with pure $ZnFe_2O_4$@MnO and $ZnFe_2O_4$@MnO –reduced graphene oxide nanocomposite, the $ZnFe_2O_4$@MnO–graphene oxide nanocomposite displayed a high photocatalytic activity on the photodegradation of Congo red. The prepared $ZnFe_2O_4$@MnO –graphene oxide nanocomposite can be potentially applied as a visible-light responsive catalyst and magnetically separable photocatalyst and thus as a powerful separation tool for solving water pollution problems.

**Keywords:** $ZnFe_2O_4$@MnO–graphene oxide nanocomposite, $ZnFe_2O_4$@MnO–reduced graphene oxide nanocomposite, Co-precipitation and hydrothermal methods, Photocatalytic activity, Congo Red Degradation.

**Acknowledgements:** We thank science and research Branch, Islamic Azad University Tehran for supporting this study and Iran Nanotechnology Initiative. And so, Thanks to Kelly Feng, CMSE2021 Conference Committee.

**CMSE4584**

## Synthesis, Characterization and Photoelectrochemical Properties of ZnO/$Fe_2O_3$, ZnO/MOF and ZnO/Biosilica Composited Films

Gabriel Yuji Hata[1*], Letícia G. da Trindade[2], Rafael Bichir Gomes de Lima Lourenço[1], José Juan Barrera-Albaa[1], Elson Longo[3], Tatiana Martelli Mazzo[1]

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**Abstract.** The necessity to diversify the global energy matrix is actual and relevant and because of that renewable resources are the key to achieve a sustainable future. In this context, the dye-sensitized solar cells (DSSCs) stand out among the electrochemical energy conversion devices since they are simple manufacturing, low cost production and eco-friendly. ZnO is a strong candidate to be used in DSSCs due to its band gap and high electron mobility. Furthermore, the photoelectrochemical properties of this oxide can be improved by the addition of dopants. In this context, ZnO particles were modified by incorporation of Hematite nanoparticles ($Fe_2O_3$), Metal–organic frameworks (MOF UiO-66-Zr) and Biosilica extracted from the marine diatom *Thalassiosira pseudonana* (BMAK 172). The pure ZnO and ZnO/MOF, ZnO/Biosilica and ZnO/ $Fe_2O_3$ composites films were studied. In this presentation, the preparation and characterization of the structural, optical and electrochemical properties of these materials will be discussed. The films were characterized by X Ray Diffraction (XRD), nitrogen adsorption–desorption isotherms, Linear Sweep Voltammetry (LSV), Chronoamperometry, Photoluminescence spectroscopy (PL), Scanning Electron Microscopy, Micro Raman and FTIR spectroscopy techniques. The photoelectrochemical measurements were made using a typical electrochemical cell system with three electrodes, a work (films prepared), a reference (Ag/AgCl) and a counter electrode (Pt) immersed in an electrolytic solution. The results demonstrated a significant increase in current density of the composite films in comparison with ZnO pure oxide film and this increased performance indicates that composite materials are promising photoelectrode for application in solar cells.

**Keywords:** ZnO, Solar, Hematite, MOF, Biosilica.

**CMSE4614**

**Preparation and Characterization of Nanocellulose and its Application**

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**Abstract.** In this work, silk- floss tree fibers were used to prepare cellulose nanofibers (CNFs) through chemical treatment and mechanical defibrillation or only through mechanical treatments. The resulting CNF's were characterized by scanning and transmission electron microscopy, x-ray diffraction and thermo- gravimetric analysis. A comparison between both preparation methods showed that it is advantageous to use the cleaner technology to obtain cellulose nanofibers.

# Part IV Poster Session

## Online Poster Presentation Guidelines

The Online Poster Presentations will consist of two parts:

- **Poster Presentations:** A collection of posters in PDF format (with/without audio) will be available at conference website for attendees to view starting on July 20, 2021.
- **Poster Q&A:** Live poster Q&A sessions will be held via Microsoft Teams Meeting for attendees to meet virtually with presenters and ask questions or give feedbacks.
- Signed and stamped electronic presentation certificate would be issued via e-mail after conference.

## List of Posters

**Time: 17:40-18:00, August 2, 2021.** Eastern European Summer Time

***Conference Room Link: http://www.academicconf.com/teamslink?confname=cmse2021***

***Should you have any questions on the posters, please feel free to write down in the notebox of each poster at CMSE2021 official website. The presenter will answer your questions as soon as possible.***

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|---|---|
| **CMSE4494** | Iterative Technique for Beams Resting on Two-Parameter Foundations Using A Refined Vlasov Model<br>*Dr. Feng Yue, School of Mechanics, Civil Engineering and Architecture, Northwestern Polytechnical University, China* |
| **CMSE4544** | Additive Remanufacturing of Coupler Knuckle based on Robotic Gas Metal Arc Welding<br>*Dr. Ziqiang Yin, Institute of Oceanographic Instrumentation, Qilu University of Technology (Shandong Academy of Sciences), China* |
| **CMSE4589** | Melt Spun of Poly(Lactic Acid) with Natural Resin Extracts: Influence of the Different Extracts on the Fiber Thermal, Mechanical, Morphological Properties<br>*PhD Evaldas Bolskis, Faculty of Mechanical Engineering and Design, Kaunas University of Technology, Lithuania* |
| **CMSE4593** | Analysis of Aging Status of Silicone Rubber Insulation Material and Research Progress of Its Repair Countermeasures<br>*Mr. Xiwei Xie, School of electrical engineering, Chongqing University, China* |
| **CMSE4606** | Colloidal Crystal Directed Block Copolymer Self-Assembled Structures<br>*Prof. Hong Kyoon Choi, Division of Advanced Materials Engineering, Kongju National University, Republic of Korea* |
| **CMSE4607** | Corrosion-Mechanical Behavior of Welded Joints of 17G1S-U Steel in the Terms Simulating Operational Conditions<br>*Dr. Nyrkova Lyudmila, E.O. Paton Electric Welding Institute of the National Academy of Sciences of Ukraine, Ukraine* |
| **CMSE4613** | Monitoring and Diagnosis System of Downhole Tubing Leakage<br>*Dr. Yunpeng Yang, China University of Petroleum-Beijing, China* |

## Abstracts of Posters

**CMSE4494 To avoid repeatability issues, this abstract will be available after the full paper is published in the conference proceedings.**

**CMSE4544 To avoid repeatability issues, this abstract will be available after the full paper is published in the conference proceedings.**

**CMSE4589**

### Melt Spun of Poly(Lactic Acid) with Natural Resin Extracts: Influence of the Different Extracts on the Fiber Thermal, Mechanical, Morphological Properties

Evaldas Bolskis[1,*], Erika Adomavičiūtė[1], Egidijus Griškonis[2], Valdas Norvydas[1]
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[2] *Faculty of Chemical Technology, Kaunas University of Technology, Radvilenu pl. 19, Kaunas, Lithuania*

**Abstract.** Melt spinning is the widely used spinning process in the textile industry. Comparing with different manufactures process of fibre, melt-spinning stands out that in this process don't needed use organic solvents. The yarns formed in this way are ideal for use in medicine field because it is possible to use additives and form multicomponent yarns with various functionalities: antimicrobial, anti-inflammatory and etc.

Poly (Lactic acid) (PLA) is an aliphatic polyester, synthesized from natural resources (most often from corn). It's is an attractive biomaterial due to good biocompatible and biodegradable with live organism. Have a good mechanical characteristic, fibre-forming ability and are widely used for medical application.

Myrrh (*Commiphora myrrh*) is a small tree. It has a range of applications and benefits for example in anti-inflammatory and many infectious diseases treatment. Myrrh resins consists of alcohol-soluble and volatile oil together with a gum soluble in water containing polysaccharides, proteins and long chain aliphatic derivatives. Their extracts have been used to cure wounds, ulcers, and different diseases of the respiratory and etc.

The aim of the research is to be developed and investigated pure PLA multifilament yarns and yarns saturated with different myrrh extract. The investigated how changed the thermal, morphological and mechanical properties using different myrrh resin extracts.

It was estimated that modification of PLA polymer with different myrrh extract have influence on thermal, morphological and mechanical properties of melt spun multifilament yarns. Melt-spun PLA yarns with aqueous myrrh extract have higher glass transition temperature $T_g$, and lower first crystallization temperature $T_{c1}$ comparing with pure PLA and PLA/Myrrh ethanol extract yarns. The

modification of PLA granules with myrrh extract influenced the mechanical properties of melt-spun yarns. The significant lower mechanical properties exhibit melt-spun yarns with aqueous myrrh extract.

**Keywords:** Myrrh, PLA, Melt spinning, Multifilament yarns.

**Acknowledgements:** Acknowledgement: E.A. and E.B. would like to acknowledge the contribution of the COST Action CA16122. E.B. would like to thank Research Council of Lithuania for funding PhD studies.

**CMSE4593 To avoid repeatability issues, this abstract will be available after the full paper is published in the conference proceedings.**

**CMSE4606**
**Colloidal Crystal Directed Block Coploymer Self-Assembled Structures**

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**Abstract.** In order to fabricate highly ordered nanopatterns using block copolymer over large area, templates for guiding the orientation of block copolymer self-assembly is essential. So far, most of directed self-assembly studies have used templates fabricated by top-dowm methods such as photo lithography or electron beam lithography. In this study, we demonstrated that another self-assembled structure, colloidal crystal, can be used as a template to guide block copolymer self-assembly. A 2D mono-layer of colloidal crystal was prepared by thermal transfer printing method from 3D self-assembled colloidal crystal having a particle size 300nm~1um. Block copolymer thin film can be coated selective area where colloidal particles were located by applying fluorine containing self-assembly monolayer on colloidal crystal template. We observed how the morphology of block copolymer changes depending on particle size and spacing of colloidal crystal template or film thickness or annealing conditions.

**Keywords:** Block copolymer, Colloidal crystal, Directed self-assembly, Nanolithography.

**CMSE4607 To avoid repeatability issues, this abstract will be available after the full paper is published in the conference proceedings.**

**CMSE4613 To avoid repeatability issues, this abstract will be available after the full paper is published in the conference proceedings.**

# Part V Acknowledgements

On behalf of the CMSE2021 Organizing Committee, we would like to take this opportunity to express our sincere gratitude to our participants. Without their support and contributions, we would not be able to hold the conference in any form. We would also like to express our acknowledgements to the Technical Program Committee members who have given their professional guidance and valuable advice as reviewers. For those who contribute to the success of the conference organization without listing the name here, we would love to say thanks as well.

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