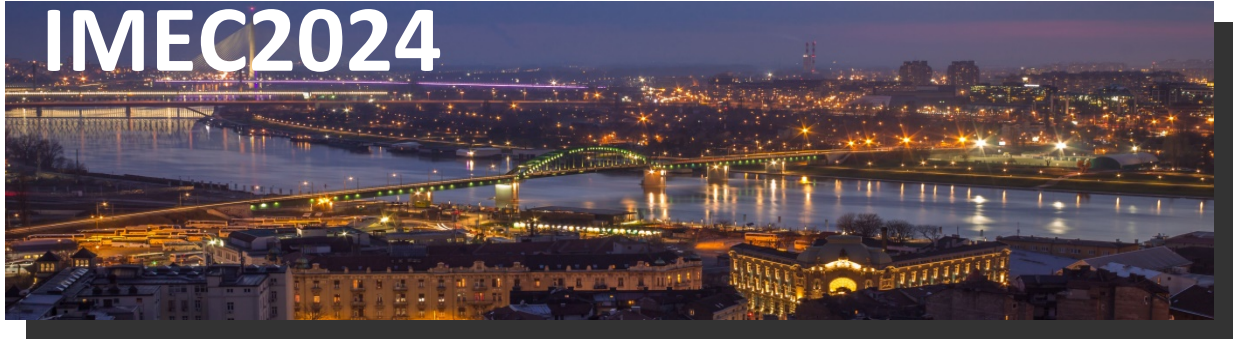


**2nd International Conference on Innovative Materials
in Extreme Conditions**



**PROGRAM
and
BOOK OF ABSTRACTS**

20-22 March 2024

Belgrade, Serbia

**2nd International Conference on Innovative Materials
in Extreme Conditions**

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and
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Program and Book of Abstracts of the 2nd International Conference on Innovative Materials in Extreme Conditions (IMEC2024) publishes abstracts from the field of material science, physics, chemistry, earth, and computational science on the phenomena arising during the processing and/or exploitation of the innovative materials, which are presented at the international conference on innovative materials in extreme conditions.

Editors-in-Chief

Dr. Rer. Nat. Branko Matović

Dr. Ivana Cvijović-Alagić

Dr. Vesna Maksimović

Dr. Dejan Zagorac

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Preface

Dear conference participants and readers, we have the pleasure to welcome you all to Belgrade, Serbia, as the venue for the 2nd International Conference on Innovative Materials in Extreme Conditions (IMEC2024). This event is jointly organized by the Serbian Society for Innovative Materials in Extreme Conditions (SIM-EXTREME), the Center of Excellence "Center for Synthesis, Processing and Characterization of Materials for Application in Extreme Conditions - CEXTREME LAB" of the Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, and the Faculty of Mechanical Engineering, University of Belgrade.

The scope of the IMEC2024 is to become the worldwide forum for discussion of experts and young researchers on the phenomena arising during the processing and/or exploitation of the innovative materials. The IMEC2024 conference is focused on the current research in the field of material science, physics, chemistry, earth, and computational science. Experimental and computational investigations of materials obtained or operated under extreme conditions presented during the conference are highlighting recent progress in the development of the innovative materials at high pressures, under high magnetic and electric fields, over a wide range of temperatures, radiation conditions, corrosive environments, under extreme mechanical loads, and non-equilibrium thermodynamic conditions. The interrelation between external effects, microstructural characteristics, and material properties is considered on the experimental and theoretical level to obtain new or enhanced insights into the material behavior and their application.

We want to use this opportunity to thank our sponsors and co-organizers for helping us to successfully organize the IMEC2024 conference. First of all, we want to mention that the Ministry of Science, Technological Development and Innovation of the Republic of Serbia recognized our conference as an important event and gave their financial endorsement. Also, we want to thank the Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, for their strong financial support. We especially appreciate the support of the Royal Family of Serbia and the Serbian Royal Palace. In the end, we would like to thank all the members of the Conference Advisory Board, the Conference International Scientific Committee, and the Conference Organizing Committee who participated in the preparations of the IMEC2024 conference.

Editors

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PROGRAM

20th March 2024

9:00 – 16:00	Conference registration (Exhibition hall)
9:20	Conference opening and Welcome address <i>Branko Matović, Conference Chair</i>
SESSION A	
Session Chairs: <i>Branko Matović, University of Belgrade, Serbia</i> <i>Ivana Cvijović-Alagić, University of Belgrade, Serbia</i>	
9:30 – 10:00	<i>Pavol Šajgalik, Slovak Academy of Sciences, Slovakia</i>
Plenary Lecture	Rapid hot-pressed silicon carbide ceramics for ultra-high temperature applications
10:00 – 10:20	<i>Tetiana Prikhna, National Academy of Sciences of Ukraine, Ukraine</i>
Invited Lecture	The high-temperature applicability of the Ti,Nb-Al-C MAX phases-based bulk materials and vacuum-arc deposited films
10:20 – 10:35	<i>Tatjana Volkov-Husović, University of Belgrade, Serbia</i>
Oral Presentation	Cavitation erosion resistance behavior of some refractory ceramics
10:35– 10:50	<i>Hakan Ünsal, Slovak Academy of Sciences, Slovakia</i>
Oral Presentation	Ablation performance of rare-earth modified ZrB ₂ -SiC composites under oxyacetylene torch test
10:50 – 11:20	Coffee break (Exhibition hall)
SESSION B	
Session Chairs: <i>Pavol Šajgalik, Slovak Academy of Sciences, Slovakia</i> <i>Tatjana Volkov-Husović, University of Belgrade, Serbia</i>	
11:20 – 11:50	<i>Miloš Đukić, University of Belgrade, Serbia</i>
Plenary Lecture	Hydrogen embrittlement in additively manufactured metals: A concise review
11:50 – 12:05	<i>Manuel Gruber, University of Leoben, Austria</i>
Oral Presentation	Mechanical testing of brittle materials: from single crystals to ceramic systems

12:05 – 12:20	<i>Bratislav Rajičić, University of Belgrade, Serbia</i>
Oral Presentation	Erosion wear of HCCI alloys
12:20 – 12:40	<i>Alexandra Kovalčíková, Slovak Academy of Sciences, Slovakia</i>
Invited Lecture	A role of micro/nano graphene platelets on strengthening and toughening mechanisms of TiB ₂ -SiC ceramic composites
12:40 – 12:55	<i>Lenka Ďaková, Slovak Academy of Sciences, Slovakia</i>
Oral Presentation	Effect of SiC whiskers on microstructure, mechanical and tribological properties of (TiZrHfNbTa)C
12:55 – 14:30	Lunch break (Conference venue)
SESSION C	
Session Chairs:	
<i>Claus Rebholz, University of Cyprus, Cyprus</i>	
<i>Nikolaos Kostoglou, University of Leoben, Austria</i>	
14:30 – 14:50	<i>Matej Fonović, University of Rijeka, Croatia</i>
Invited Lecture	Growth and stability of Ni ₃ N layers obtained in pure ammonia at high temperatures
14:50 – 15:05	<i>Zoltán Lenčéš, Slovak Academy of Sciences, Slovakia</i>
Oral Presentation	Atomic layer deposition assisted graphite/ZnO composite anodes in Li-ion batteries
15:05 – 15:20	<i>Marko Jelić, University of Belgrade, Serbia</i>
Oral Presentation	Physicochemical properties of bismuth vanadate photoanode irradiated by swift heavy ions
15:20 – 15:35	<i>Željko Mravik, University of Belgrade, Serbia</i>
Oral Presentation	Utilization of swift heavy ions for modification of graphene oxide-based nanocomposites
15:35 – 15:50	<i>Ondrej Hanzel, Slovak Academy of Sciences, Slovakia</i>
Oral Presentation	Thermal and electrical conductivity of additive-free silicon carbide ceramics
16:00 – 18:00	Poster Session (Exhibition hall)
18:00	Welcome reception (Conference venue)

21st March 2024

SESSION D	
Session Chairs: <i>Alexandra Kovalčíková, Slovak Academy of Sciences, Slovakia</i> <i>Zoltán Lenčėš, Slovak Academy of Sciences, Slovakia</i>	
09:30 – 09:50 Invited Lecture	<i>Subramshu Shekar Bhattacharya, Indian Institute of Technology - Madras, India</i> Order amidst disorder in multicomponent high entropy oxides (HEOs): synthesis, characterization and applications
09:50 – 10:10 Invited Lecture	<i>Peter Tatarko, Slovak Academy of Sciences, Slovakia</i> Development and Integration of Entropy Stabilized Ceramics
10:10– 10:25 Oral Presentation	<i>Dharma Teja Teppala, Technical University of Darmstadt, Germany</i> Synthesis and high-temperature/high-pressure exposure of compositionally complex rock-salt-type transitional metal (carbo)nitrides
10:25 – 11:00	Coffee break (Exhibition hall)
SESSION E	
Session Chairs: <i>Tetiana Prikhna, National Academy of Sciences of Ukraine, Ukraine</i> <i>Dejan Zagorac, University of Belgrade, Serbia</i>	
11:00 – 11:30 Plenary Lecture	<i>Miladin Radović, Texas A&M University, USA</i> MAX Phases: Overcoming the challenges of extreme environments
11:30 – 12:30	Lunch break (Conference venue)
12:30 – 15:00	Guided visit to White Palace (the official residence of the former Yugoslav royal family)
20:00	Conference gala dinner Restaurant Caruso <i>Address: Terazije 23/8, Belgrade</i>

22nd March 2024

SESSION F	
Session Chairs:	
<i>Miladin Radović, Texas A&M University, USA</i>	
<i>Miloš Đukić, University of Belgrade, Serbia</i>	
9:30 – 10:00	<i>Ravi Kumar, Indian Institute of Technology - Madras, India</i>
Plenary Lecture	Small-scale mechanical testing of entropy stabilized ceramics
10:00 – 10:20	<i>Shanti Bhattacharya, Indian Institute of Technology - Madras, India</i>
Invited Lecture	Nano and micro optics on fibre tip: A possible solution for measurements in harsh environments
10:20 – 10:35	<i>Muniyappa Amarnath, Indian Institute of Information Technology Design and Manufacturing, India</i>
Oral Presentation	Experimental investigations to evaluate surface fatigue wear in journal bearing by using vibration signal analysis
10:35 – 10:50	<i>Ramachandra C G, Presidency University, India</i>
Oral Presentation	Experimental and simulation analysis of influence of stacking sequence on tensile and abrasion resistance of e-glass/jute fibre-based hybrid composites
10:50 – 11:20	Coffee break (Exhibition hall)
SESSION G	
Session Chairs:	
<i>Hari Kumar, Indian Institute of Technology - Madras, India</i>	
<i>Peter Tatarko, Slovak Academy of Sciences, Slovakia</i>	
11:20 – 11:40	<i>Maria Čebela, University of Belgrade, Serbia</i>
Invited Lecture	Enhancement of weak ferromagnetism, exotic structure prediction and diverse electronic properties in bismuth ferrite and holmium-substituted multiferroic bismuth ferrite
11:40 – 11:55	<i>Dejan Zagorac, University of Belgrade, Serbia</i>
Oral Presentation	Study of lanthanum fluoride selenides using a combination of crystal structure prediction and DFT calculations with experimental synthesis and characterization
11:55 – 12:10	<i>Dušica Jovanović, University of Niš, Serbia</i>
Oral Presentation	DFT study of new hybrid organic-inorganic perovskites: guanidinium-BX ₃ substituted by B = (Sr ²⁺ , Ca ²⁺ , Mg ²⁺ , Be ²⁺) and X = (Cl ⁻ , F ⁻)

12:10 – 12:30	<i>Thomas Bräuniger, Ludwig-Maximilians-University of Munich, Germany</i>
Invited Lecture	NMR spectroscopy as a structure elucidation tool for compounds synthesised under high temperature and high pressure conditions
12:30 – 14:00	Lunch break (Conference venue)
14:00	Conference closing ceremony

DFT study of new hybrid organic-inorganic perovskites: guanidinium-BX₃ substituted by B = (Sr²⁺, Ca²⁺, Mg²⁺, Be²⁺) and X = (Cl⁻, F⁻)

Dušica Jovanović^{1,2}, Dejan Zagorac^{1,3}, J. Christian Schön⁴, Branko Matović^{1,3}, Aleksandra Zarubica², Jelena Zagorac^{1,3}

¹*Institute of Nuclear Sciences Vinča, Materials Science Laboratory, University of Belgrade, 11000 Belgrade, Serbia*

²*Department of Chemistry, Faculty of science and mathematics, University of Nis, 18000 Nis, Serbia*

³*Center for Synthesis, Processing and Characterization of Materials for Application in the Extreme Conditions-CextremeLab, 11000 Belgrade, Serbia*

⁴*Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany*

In recent years, the development of perovskite solar cells (PSC) has attracted great attention as a “green” energy source that might even replace fossil fuels soon [1]. Conventional perovskite solar cells mostly contain toxic lead, which contributes to environmental pollution, so the solution was found to substitute lead with some non-toxic metal [2]. Our investigation of hybrid organic-inorganic perovskites aims to increase the chemical stability as well as to decrease the band gap value of crystal perovskites which enables better conductivity and shifts the absorbance range, in order to produce the most efficient perovskite solar cells. The *ab initio* calculations of GA-BX₃, where GA is the guanidinium cation C(NH₂)₃⁺, with several different inorganic cations and anions - specifically: B = (Sr²⁺, Ca²⁺, Mg²⁺, Be²⁺) and X = (Cl⁻, F⁻) have been performed using Density Functional Theory (DFT), with several functionals, Local Density Approximation (LDA) and Perdew-Burke-Ernzerhof (PBE), as well as HSE06 (Heyd-Scuseria-Ernzerhof) hybrid functional. Further investigations of structural and electronic properties will provide insights into the potential applications of these new hybrid organic-inorganic perovskite structures.

References:

- [1] C.C. Stoumpos, Journal of the American Chemical Society 137 (2015) 6804–6819.
[2] C.C. Stoumpos, Inorganic Chemistry 56 (2017) 56–73.

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