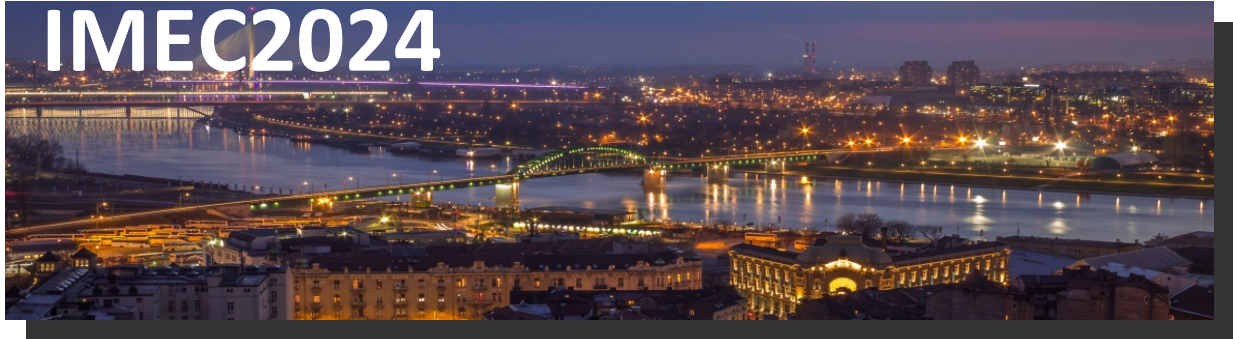


**2<sup>nd</sup> International Conference on Innovative Materials  
in Extreme Conditions**



**PROGRAM  
and  
BOOK OF ABSTRACTS**

**20-22 March 2024**

**Belgrade, Serbia**

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in Extreme Conditions**

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**Program and Book of Abstracts of the 2<sup>nd</sup> 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

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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 2<sup>nd</sup> 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**

**20<sup>th</sup> March 2024**

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



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

**21<sup>st</sup> March 2024**

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

22<sup>nd</sup> March 2024

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

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

## Theoretical Investigations of Electronic Properties of Predicted Y<sub>2</sub>O<sub>2</sub>S

**Dragana Jordanov<sup>1</sup>, Dejan Zagorac<sup>1</sup>, Klaus Doll<sup>2</sup>, Johann Christian Schön<sup>3</sup>, Milena Rosić<sup>1</sup>,  
Maria Čebela<sup>1</sup>**

<sup>1</sup>*Vinča "Institute of Nuclear Science, National Institute of the Republic of Serbia, University of  
Belgrade, Belgrade, Serbia*

<sup>2</sup>*Institute for Theoretical Chemistry, University of Stuttgart, Stuttgart, Germany*

<sup>3</sup>*Nanoscale Science Department, Max Planck Institute for Solid State Research, 70569 Stuttgart,  
Germany*

Rare-earth Oxysulfides have many applications such as solar energy, wind turbines, batteries for electric vehicles and mobile phones, cathode ray tubes, metal alloys, ceramic materials and so on. In this study we perform crystal structure prediction and investigate energy landscape of Yttrium Oxysulfide (Y<sub>2</sub>O<sub>2</sub>S). Global optimizations on the energy landscape of Y<sub>2</sub>O<sub>2</sub>S have been carried out using empirical potentials followed by, a local optimization using *ab initio* calculations [1]. Our calculations showed the *Alpha* phase in good agreement with the experimentally observed trigonal structure. Furthermore, novel *Beta* and *Gamma* modifications of pure Yttrium Oxysulfide have been discovered. Y<sub>2</sub>O<sub>2</sub>S is a material known as a wide-gap semiconductor. From the calculation of the bulk, it is found that the material has an indirect band gap and that the top of the valence bands shows an anisotropic character which means an anisotropic mass of the hole [2]. We included the calculation of the Density of States (DOS) for the most stable structures (*Alpha*, *Beta* and *Gamma*) and discuss the band gaps, also [3]. The results presented here have all been performed using the B3LYP functional and local density approximation (LDA). Our calculations are in good agreement with the literature data [4].

### References

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