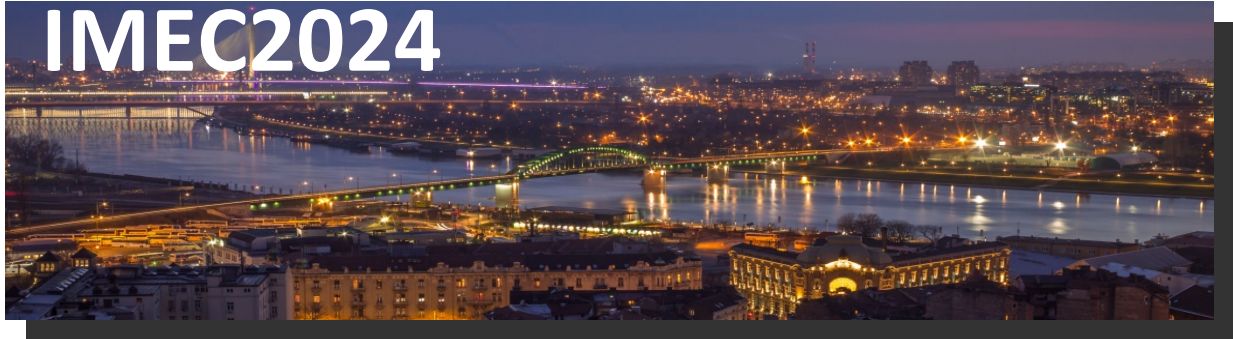


**2<sup>nd</sup> International Conference on Innovative Materials  
in Extreme Conditions**



**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.

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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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## TABLE OF CONTENTS

<b>PROGRAM</b> .....	14
20 <sup>th</sup> March 2024 .....	15
21 <sup>st</sup> March 2024 .....	17
22 <sup>nd</sup> March 2024 .....	18
 <b>PLENARY LECTURES</b> .....	 20
 <i>Pavol Šajgalik, Ondrej Hanzel, Michal Hičák, Alexandra Kovalčíková, Chengyu Zhang, Alexander Mukasyan</i>	
Rapid hot-pressed silicon carbide ceramics for ultra-high temperature applications.....	21
 <i>Miloš Đukić, Alireza Behvar, Meysam Haghshenas, Gordana M. Bakić, Dejan Zagorac, Aleksandar Sedmak, Bratislav Rajičić</i>	
Hydrogen embrittlement in additively manufactured metals: A concise review .....	22
 <i>Miladin Radović</i>	
MAX Phases: Overcoming the challenges of extreme environments.....	23
 <i>Ravi Kumar</i>	
Small-scale mechanical testing of entropy stabilized ceramics .....	24
 <b>INVITED LECTURES</b> .....	 25
 <i>Tetiana Prikhna, T.B. Serbenyuk, O.P. Ostash, V.B. Sverdun, A.S. Kuprin, B. Matović, I. Cvijović-Alagić, V.Ya. Podhurska</i>	
The high-temperature applicability of the Ti,Nb-Al-C MAX phases-based bulk materials and vacuum-arc deposited films .....	26
 <i>Alexandra Kovalčíková, P. Tatarko, Z. Chlup, R. Sedlák, E. Múdra, J. Dusza</i>	
A role of micro/nano graphene platelets on strengthening and toughening mechanisms of TiB <sub>2</sub> -SiC ceramic composites .....	27
 <i>Matej Fonović, Dario Kvrčić</i>	
Growth and stability of Ni <sub>3</sub> N layers obtained in pure ammonia at high temperatures .....	28
 <i>Subramshu Shekar Bhattacharya</i>	
Order amidst disorder in multicomponent high entropy oxides (HEOs): synthesis, characterization and applications .....	29

<i>Peter Tatarko, Naser Hosseini, Fabrizio Valenza, Hakan Ünsal, Zdeněk Chlup, Alexandra Kovalčíková, I. Dlouhý</i> Development and integration of entropy stabilized ceramics .....	30
<b>Shanti Bhattacharya</b> Nano and micro optics on fibre tip: A possible solution for measurements in harsh environments .....	31
<i>Maria Čebela, Vitalii Turchenko, Milena Rosić, Dragana Jordanov, Vladimir Dodevski, Dejan Zagorac</i> Enhancement of weak ferromagnetism, exotic structure prediction and diverse electronic properties in bismuth ferrite and holmium-substituted multiferroic bismuth ferrite .....	32
<b>Thomas Bräuniger</b> NMR spectroscopy as a structure elucidation tool for compounds synthesised under high temperature and high pressure conditions .....	33
<b>ORAL PRESENTATIONS</b> .....	34
<i>Tatjana Volkov-Husović, Sanja Martinović, Ana Alil</i> Cavitation erosion resistance behavior of some refractory ceramics .....	35
<i>Hakan Ünsal, Alexandra Kovalčíková, Michal Hičák, Zdenek Chlup, Ivo Dlouhý, Branko Matović, Peter Tatarko</i> Ablation performance of rare-earth modified ZrB <sub>2</sub> -SiC composites under oxyacetylene torch test .....	36
<i>Manuel Gruber, Peter Supancic, Raul Bermejo</i> Mechanical testing of brittle materials: from single crystals to ceramic systems .....	37
<i>Bratislav Rajičić, Aleksandar Maslarević, Gordana Bakić, Vesna Maksimović, Miloš Đukić</i> Erosion wear of HCCI alloys .....	38
<i>Lenka Ďaková, Monika Hrubovčáková, Alexandra Kovalčíková, Jana Andrejovská, Ján Dusza</i> Effect of SiC whiskers on microstructure, mechanical and tribological properties of (TiZrHfNbTa)C .....	39
<i>Alper Güneren, Prangya P. Sahoo, Boris Hudec, Matej Mičušík, Zoltán Lenčేశ, Karol Fröhlich</i> Atomic layer deposition assisted graphite/ZnO composite anodes in Li-ion batteries.....	40
<i>Marko Jelić, Ekaterina Korneeva, Nikita Kirilki, Tatiana Vershinin, Oleg Orelovich, Vladimir Skuratov, Zoran Jovanović, Sonja Jovanović</i> Physicochemical properties of bismuth vanadate photoanode irradiated by swift heavy ions	41

<i>Željko Mravik, Milica Pejčić, Danica Bajuk-Bogdanović, Nikita Kirilkin, Ekaterina Korneeva, Vladimir Skuratov, Zoran Jovanović</i>	
Utilization of swift heavy ions for modification of graphene oxide-based nanocomposites	42
<i>Ondrej Hanzel, Monika Tatarková, Pavol Šajgalik</i>	
Thermal and electrical conductivity of additive-free silicon carbide ceramics.....	43
<i>Dharma Teja Teppala, Shrikant Bhat, Leonard Keil, Jan Bernauer, Johannes Peter, Hans-Joachim Kleebe, Emanuel Ionescu</i>	
Synthesis and high-temperature / high-pressure exposure of compositionally complex rock-salt-type transitional metal (carbo)nitrides .....	44
<i>Muniyappa Amarnath, Ramachandra C G, H. Chelladurai, P. Sateesh Kumar, K. Santhosh Kumar</i>	
Experimental investigations to evaluate surface fatigue wear in journal bearing by using vibration signal analysis .....	45
<i>Ramachandra C G, Lokesh K S, Srinivasa Mayya D, Ravindra Babu G</i>	
Experimental and simulation analysis of influence of stacking sequence on tensile and abrasion resistance of e-glass/jute fibre-based hybrid composites .....	46
<i>Dejan Zagorac, Constantin Buyer, Jelena Zagorac, Hagen Grossholz, Sarah Wolf, Tamara Škundrić, Milan Pejić, Dušica Jovanović, J. Christian Schön, Thomas Schleid</i>	
Study of lanthanum fluoride selenides using a combination of crystal structure prediction and DFT calculations with experimental synthesis and characterization .....	47
<i>Dušica Jovanović, Dejan Zagorac, J. Christian Schön, Branko Matović, Aleksandra Zarubica, Jelena Zagorac</i>	
DFT study of new hybrid organic-inorganic perovskites: guanidinium-BX <sup>3</sup> 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> ).....	48
<b>POSTER PRESENTATIONS</b> .....	49
<i>Ivana Cvijović-Alagić, Nikola Kanas, Jelena Maletaškić, Abishek M, Vesna Maksimović</i>	
Novel high entropy alloys for extreme environments .....	50
<i>Vesna Maksimović, Vladimir Urbanovich, Jelena Maletaškić, Vladimir Pavkov, Ivana Cvijović-Alagić</i>	
Characterization of the high-pressure sintered TiAl-TiB <sub>2</sub> composites.....	51
<i>Nikolaos Kostoglou, Christos Tampaxis, Georgia Charalambopoulou, Georgios Constantinides, Vladislav Ryzhkov, Charalabos Doumanidis, Branko Matović, Christian Mitterer, Claus Rebholz</i>	
Boron nitride nanotubes versus carbon nanotubes: A thermal stability and oxidation behavior study .....	52

<i>Nikolaos Kostoglou, Sebastian Stock, Angelos Solomi, Damian Holzappel, Steven Hinder, Mark Baker, Georgios Constantinides, Vladislav Ryzhkov, Jelena Maletaškić, Branko Matović, Jochen Schneider, Claus Rebholz, Christian Mitterer</i> Purity and surface area: Key factors on thermal stability and oxidation resistance of BN nanoplatelets.....	53
<i>Anna Kityk, Miroslav Hnatko, Viliam Pavlik, Michal Hičák</i> Sustainable Solutions in Biomedical Substrate Design: Micro- and Nanotexturing on 3D Printed Titanium Alloys .....	54
<i>Tetiana Prikhna, Pavlo Barvitskyi, Branko Matović, Dejan Zagorac, Anastasiya Lokatkina, Bernd Büchner, Jochen Werner, Myroslav Karpets, Robert Kluge, Viktor Moshchil, Anatolii Bondar, Olexander Borymskyi, Leonid Devin, Semyon Ponomarov</i> Structure, mechanical characteristics and high-temperature stability of sintered under high and by hot pressing ZrB <sub>2</sub> - and HfB <sub>2</sub> -based composites.....	55
<i>Tamara Škundrić, Johann Christian Schön, Aleksandra Zarubica, Matej Fonović, Milan Pejić, Jelena Zagorac, Dejan Zagorac</i> Energy landscape exploration of the novel CrSi <sub>2</sub> N <sub>4</sub> compound .....	56
<i>Ivana Cvijović-Alagić, Jelena Maletaškić, Vladimir Pavkov, Slaviša Putić, Branko Matović, Vesna Maksimović</i> Enhanced aluminum matrix composites for structural applications.....	57
<i>Maria Čebela, Nataša Tomić, Milica Vujković, Milena Rosić, Vesna Lojpur</i> Two different paths to obtain pure nanosized Fe <sub>3</sub> O <sub>4</sub> : Morphology and Magnetic properties .....	58
<i>Dragana Jordanov, Dejan Zagorac, Klaus Doll, Johan Christian Schön, Milena Rosić, Maria Čebela</i> Theoretical Investigations of Electronic Properties of Predicted Y <sub>2</sub> O <sub>2</sub> S.....	59
<i>Bratislav Todorović, Dragan Stojiljković, Tanja Petrović Pantić</i> Carbonate compounds formed by degassing of geothermal water from borehole B-4 at Sijarinska Banja (Serbia).....	60
<i>Marija Egerić, Dimitrije Petrović, Marjetka Savić, Aleksandar Devečerski, Srboljub Stanković, Radojka Vujasin, Ljiljana Matović</i> Gamma Irradiation Induced Dyes Degradation: Recent Progress and Future Perspective for Wastewater Treatment.....	61
<i>Tetiana Prikhna, Aiswarya Kethamkuzhi, Roxana Vlad, Branko Matović, Semyon Ponomarov, Robert Kluge, Myroslav Karpets, Viktor E. Moshchil, Xavier Obradors, Joffre Gutierrez, Bernd Büchner, Teresa Puig</i> Characterization of high pressure oxygenated EuBCO and GdBCO coated conductors.....	62

<b>Tijana Stamenković, Maria Čebela, Milena Rosić, Vesna Lojpur</b> Photocatalytic application of SrGd <sub>2</sub> O <sub>4</sub> nanoparticles doped with rare earth.....	63
<b>Milena Rosić, Maja Milošević, Vladimir Dodevski, Dragana Jordanov, Vesna Lojpur, Tijana Vlašković, Maria Čebela</b> Spectroscopic and Morphological Properties of Co <sub>0.9</sub> Ho <sub>0.1</sub> MoO <sub>4</sub> nanopowders.....	64
<b>Marko Simić, Jovana Ružić, Dušan Božić, Željko Radovanović, Jelena Stašić</b> Mechanical alloying as a crucial step in the fabrication process of Cu alloys .....	65
<b>Tijana B. Vlašković, Bojana Laban, Maria Čebela, Vladimir Dodevski, Dragana Jordanov, Milena Rosić</b> Preparation of Ca <sub>0.9</sub> Er <sub>0.1</sub> MnO <sub>3</sub> nanopowders by combustion method.....	66
<b>Ružica Mihailović, Aleksandra Zarubica, Branko Matović, Svetlana Butulija</b> Activating agricultural residues: Corn cob as a resource for adsorption-based pollution management .....	67
<b>Vladimir Pavkov, Gordana Bakić, Vesna Maksimović, Ivana Cvijović-Alagić, Aleksandar Maslarević, Bratislav Rajičić, Nenad Milošević</b> The influence of stainless steel particles reinforcement on the fracture toughness of glass-ceramic matrix composite .....	68
<b>Jana Andrejovská, Ondrej Petruš, Dávid Medved', Marek Vojtko, Marcel Riznič, Peter Kizek, Ján Dusza</b> Mechanical properties of human enamel and dentin: a study by nanoindentation.....	69
<b>Dejan Zagorac, Jelena Zagorac, Matej Fonović, Tamara Škundrić, Milan Pejić, Dušica Jovanović, Miloš B. Đukić, Branko Matović</b> Structure-property relationship of AlN/BN mixed compounds on DFT level.....	70
<b>Dávid Medved', Jana Andrejovská, Marek Vojtko, Annamária Naughton-Duszová, Piotr Klimczyk</b> Nanoindentation Properties of Al <sub>2</sub> O <sub>3</sub> + ZrO <sub>2</sub> + WTiC/ZrC Ceramics Fabricated by SPS...	71
<b>Jelena Zagorac, Dušica Jovanović, Dejan Zagorac, Tamara Škundrić, Milan Pejić, Vesna Šrot, Branko Matović</b> Multidisciplinary approach in investigating ZnO/ZnS core/shell nanostructures.....	72
<b>Svetlana Butulija, Jelena Filipović Tričković, Ana Valenta Šobot, Bratislav Todorović, Sanja Petrović, Bojana Ilić, Danica Zmejkoski, Branko Matović</b> Bacterial Cellulose-Cerium Oxide Hydrogel for Tailored Redox Balance in Biomedical Extremes.....	73
<b>Marija Prekajski Đorđević, Jelena Maletaškić, Svetlana Butulija, Emilija Nidžović, Aleksa Luković, Ravi Kumar, Branko Matović</b> High-entropy stabilized Zr <sub>0.2</sub> Hf <sub>0.2</sub> Ce <sub>0.2</sub> Yb <sub>0.2</sub> Gd <sub>0.2</sub> O <sub>2-δ</sub> with fluorite structure.....	74

<i>Aleksa Luković, Diana Carolina Lago, Jozef Kraxner, Dušan Galusek, Branko Matović, Danica Srećković-Batočanin, Jelena Maletaškić</i> Basaltic Glass-Ceramic Composites: Exploring Structural, Morphological, and Thermal Insights for Ballistic Protection and Radiation Shielding Applications.....	75
<i>Milan Pejić, Dejan Zagorac, Jelena Zagorac, Tamara Škundrić, Dušica Jovanović, Branko Matović</i> Energy Landscape Exploration of Novel Rare Earth Chalcohalides LaXY (X=O,S; Y=I,F).....	76
<i>Tamara Minović Arsić, Jelena Maletaškić, Svetlana Butulija, Emilija Nidžović, Jelena Erčić, Marija Prekajski Đorđević, Branko Matović</i> Synthesis and characterization of ceria doped with mercury.....	77
<i>Jelena Maletaškić, Yulia Gorshkova, Sergei Yurievich Kottsov, G.P. Kopitsa, Branko Matović</i> SAXS characterization of morphology controlled nano ceria.....	78
<b>AUTHOR INDEX</b> .....	79

# **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>

## Energy landscape exploration of the novel CrSi<sub>2</sub>N<sub>4</sub> compound

**Tamara Škundrić<sup>1,2</sup>, Johann Christian Schön<sup>3</sup>, Aleksandra Zarubica<sup>4</sup>, Matej Fonović<sup>5</sup>, Milan Pejić<sup>1,2</sup>, Jelena Zagorac<sup>1,2</sup>, Dejan Zagorac<sup>1,2</sup>**

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The Cr-Si-N system holds significant importance for materials exhibiting advanced tribological and mechanical properties. Previous research has focused on Cr-Si-N coating, nanocrystalline phases, thin films, as well as theoretically predicted 1D and 2D hetero-structures, and 3D bulk Cr<sub>2</sub>SiN<sub>4</sub> modifications. This particular study aims to predict potential bulk Cr-Si-N phases, specifically with the composition CrSi<sub>2</sub>N<sub>4</sub>. The research employs a multi-methodological approach, combining global optimization with data mining and the Primitive Cell for Atom Exchange (PCAE) method to explore the energy landscape of the system. Local optimization of structure candidates is conducted at the Density Functional Theory (DFT) level using the GGA-PBE and the LDA-PZ approximation. Among the discovered structure candidates in the CrSi<sub>2</sub>N<sub>4</sub> chemical system, the ten most energetically favorable ones predominantly display monoclinic symmetry. However, these structures exhibit a range of features, from zeolite-like structures to polytypic behavior. The study also involved computing the bulk modulus and cell volume of all predicted CrSi<sub>2</sub>N<sub>4</sub> phases under various pressures, extending up to 10 GPa. Additionally, the decomposition of CrSi<sub>2</sub>N<sub>4</sub> into CrN, Si<sub>3</sub>N<sub>4</sub>, and N<sub>2</sub> has been investigated and the results suggested that the TiMn<sub>2</sub>O<sub>4</sub>-type modification, identified as the global minimum phase, should remain stable, particularly at lower temperatures. Given the absence of experimental data for comparison, the study employed two different functionals to assess the robustness of the energy ranking and structural data. The good agreement observed between the two calculation levels suggests a high likelihood that the identified structure candidates represent actual (meta)stable modifications for bulk CrSi<sub>2</sub>N<sub>4</sub>. This discovery offers promising targets for future experimental synthesis, opening avenues for further theoretical studies on the electronic and magnetic properties of these materials.

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