



# Twenty-fifth Jubilee Annual Conference

Thirteenth World Round Table Conference on Sintering

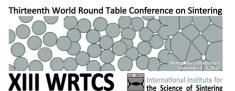
**IWRTGS** 

# Program and Book of Abstracts

endorsed by FEENS FEDERATION OF EUROPEAN MATERIALS SOCIETIES







### TWENTY-FIFTH JUBILEE ANNUAL CONFERENCE ON MATERIAL SCIENCE YUCOMAT 2024

&

### THIRTEENTH WORLD ROUND TABLE CONFERENCE ON SINTERING XIII WRTCS 2024

Hunguest Hotel Sun Resort, Herceg Novi, Montenegro September 2 to 6, 2024

## Program and Book of Abstracts

Organised by Materials Research Society of Serbia & International Institute for the Science of Sintering

Endorsed by Federation of European Material Societies CIP - Каталогизација у публикацији Народна библиотека Србије. Београд 66.017/.018(048) 621.762.5(048) DRUŠTVO za istraživanje materijala Srbije (Beograd). Godišnja konferencija (25; 2024; Herceg Novi) Programme ; and The Book of Abstracts / Twenty-fifth Jubilee Annual Conference YUCOMAT 2024 & Thirteenth World Round Table Conference on Sintering XIII WRTCS 2024, Herceg Novi, Montenegro, September 2 to 6, 2024 ; organised by Materials Research Society of Serbia & International Institute for the Science of Sintering : leditor Dragan P. Uskokovići. - Belgrade : Materials Research Society of Serbia, 2024 (Herceg Novi : Biro Konto), - XL, 169 str. : ilustr. : 23 cm Tiraž 220. - Bibliografija uz pojedine apstrakte. - Registar. ISBN 978-86-919111-9-5 1. World Round Table Conference on Sintering (13; 2024; Herceg Novi) а) Наука о материјалима -- Апстракти b) Технички материјали -- Апстракти v) Синтеровање --Апстракти COBISS.SR-ID 150427657

25th JUBILEE ANNUAL CONFERENCE ON MATERIAL SCIENCE YUCOMAT 2024 13th WORLD ROUND TABLE CONFERENCE ON SINTERING XIII WRTCS 2024 Herceg Novi, Montenegro, September 2 to 6, 2024

#### **Program and Book of Abstracts**

Publisher:	Materials Research Society of Serbia Knez Mihailova 35/IV, P. O. Box 433, 11000 Belgrade, Serbia Phone: +381 11 2185-437; <u>http://www.mrs-serbia.org.rs</u>
Editor:	Prof. Dr. Dragan P. Uskoković
Technical editors:	Dr. Sonja Jovanović and Dr. Ivana Dinić
Typesetting and prepress: Dr. Aleksandar Dekanski	
Covers:	Front cover photo: J. Erskine-Kelli, Attribution-ShareAlike 2.0 Generic (CC BY-SA 2.0) Back cover photo: property of MRS Serbia
ISBN 978-86-919111-9-5	

https://doi.org/10.5281/zenodo.13303138

**Copyright**<sup>©</sup> 2024 Materials Research Society of Serbia – MRS Serbia

MRSS is member of the Federation of European Materials Societies



Printed in: Biro Konto, Sutorina bb, Igalo - Herceg Novi, Montenegro Phones: +382-31-670123, 670025, E-mail: bkonto@t-com.me

Circulation: 220 copies. The end of printing: August 2024

## CONTENTS

Welcome speech by the President of MRS-Serbia	_ v
2024 MRS-SERBIA Award for a Lasting and Outstanding Contribution to Materials Science and Engineering	
MATERIALS RESEARCH SOCIETY OF SERBIA	_ix
INTERNATIONAL INSTITUTE FOR THE SCIENCE OF SINTERING	_ x
YUCOMAT 2024 & XIII WRTCS committees	_xi
General information	_xi
GENERAL YUCOMAT 2024 & XIII WRTCS PROGRAM	xiii
SCIENTIFIC YUCOMAT 2024 & XIII WRTCS PROGRAM	_xv
ABSTRACTS YUCOMAT Plenary Lectures	_ 1
YUCOMAT Oral Presentations	17
YUCOMAT Poster Presentations	49
WRTCS Plenary Lectures	
WRTCS Oral Presentations	
WRTCS Poster Presentations	153
Author Index	165

#### WELCOME SPEECH BY THE PRESIDENT OF MRS-SERBIA

#### Esteemed Colleagues, Fellow Scientists and Honored Guests,



It is my great pleasure to greet you on behalf of the International Institute for the Science of Sintering (www.iisssci.org) and the Materials Research Society of Serbia (www.mrsserbia.org.rs) at this jubilee event marking 55 years since the First Conference of the International Institute for the Science of Sintering, held in July 1969 at this hotel. This conference is dedicated to the founders of the Institute, Prof. Momčilo M. Ristić, long-time General Secretary and President of the Institute from Belgrade, and Drago Kolar, professor at the University of Ljubljana and scientific advisor at the Jožef Stefan Institute. The other celebrant is the Materials Research Society of Serbia, which

held its First Inaugural Conference in September 1995 and all subsequent ones in Herceg Novi. This is the 25<sup>th</sup> Conference, as they were initially held every other year, transitioning to an annual conference in 2003. I also wish you a good program and many pleasant gatherings, which have always been the hallmark of these Conferences.

I remember that first Conference on Sintering, attended by leading figures in the field: George Kuczynski, Robert L. Coble, David Lynn Johnson, Helmut Fischmeister, Fritz Thummler, Yakov Evseevich Geguzin, Ivan Mihailovich Fedorchenko, and many others. Financial support for their arrival and stay was provided by the leading ceramics and sinter-metallurgy industries of Yugoslavia: Electronics Industry - Niš and Belgrade, Magnohrom - Kraljevo, Prvi Partizan - Titovo Užice, Energoinvest - Sarajevo. After the Conference, they visited the factories that financed their participation, gave lectures, and had fruitful discussions with their associates. Today it is completely different, and I can't recall the last time an industry associate participated in our YUCOMAT and Sintering Conferences. Times have changed, and wartime and post-war events and the privatization of our economy have completely changed the overall picture, so we no longer have this type of science-industry collaboration.

This year's YUCOMAT 2024 and XIII Sintering Conference programs include 5 Plenary sessions (3 at YUCOMAT with 12 plenary lectures and 2 at Sintering with 9 plenary lectures). While all plenary speakers accepted the invitation to speak at Sintering, a significant number postponed their participation in YUCOMAT for the next year (September 1-5, 2025) for justified reasons. As in recent years, the plenary lectures set these Conferences apart from many others in the world: exceptionally high positions on the world citation lists of plenary lecturers (this time 4 of the top 100, and nearly all have an h-index above 100). The WRTCS plenary lecturers are certainly the most successful in their field. Of the 150 oral and poster presentations from 23 countries, the most are from Serbia (40 %), followed by Ukraine (20 %), Poland (8 %), Czech Republic (6 %), Montenegro (4 %), Slovenia (3.3 %), and Spain (2.6 %). It is noticeable that participation from EU authors is significantly lower than in previous years.

This year's recipient of the Award of the Materials Research Society of Serbia, for lasting and outstanding contributions to materials science and engineering, is Prof. Vladimir Torchilin for his enormous contributions in pharmaceutical biotechnology and nano-medicine. He is the founder and director of the Center of the same name at Northeastern University in Boston, holds numerous accolades, is a member of the International Program Committees, and a speaker at many worlds and our Conferences. His works have been cited numerous times with an *h*-index of 133, 94,000 citations, and 64 patents, placing him in the top category of researchers. All data are in this year's Program and Abstract Book. Prof. Torchilin is here, and after the ceremonial opening, he will speak on the topic "Stimuli-sensitive drug delivery system".

This is the third WRTCS Conference held together with YUCOMAT after 15 years of inactivity, following the decision of the Institute's Board of Directors to renew its work. Significant progress is already noticeable. New members have been elected, so now there are 93 actives, out of 183 elected so far. We have created a nice website where all information is timely updated. Year after year, the number of papers at WRTCS increases, and this year there will be about thirty, including 9 plenary lectures. Just before the Conference, from August 30 to September 1, three IISS members (Prof. Suk-Joong L. Kang - KAIST, Prof. Eugene A. Olevsky - San Diego State University, and Prof. Vincenzo Sglavo - University of Trento) held an 18-hour Tutorial for young researchers. The Managing Board's suggestion to start awarding Institute Prizes to encourage greater activity among members was honored, and after 22 years, it was decided to award the Frenkel Prize "for extraordinary contributions to the Science of Sintering" to two of our most distinguished and active members this year.

This year, for the third consecutive time, Drexel University, in collaboration with EOARD and MRS-Serbia, supported 21 participants from Ukraine, covering their Conference fee and accommodation at the Hunguest Sun Resort Hotel.

Many participants from around the world have spoken at these Conferences over the past 55 years. Since the First Conference on Sintering held in 1969, despite a fifteen-year break (2002-2017), more than 2500 lectures have been held here in Herceg Novi, in cities of the former Yugoslavia (Dubrovnik, Portorož, Belgrade), and across Europe, North America, and the Far East (Warsaw, New Delhi, Tokyo, Vancouver) by experts who scientifically and technologically formed this field. In the 25 Conferences of the Materials Research Society of Serbia, more than 4500 lectures have been held here in Herceg Novi by authors from over 60 countries, including more than 450 plenary lectures by the most successful scientists in new materials and nanotechnology, including Nobel Prize winners and those seriously vying for it. Now they represent a whole, where they complement each other program- and content-wise, and represent our country and its science to the world with dignity.

In conclusion, I wish you a good program, new contacts, and that you leave Herceg Novi happily and satisfied, and return many more times.

> MRS Serbia and IISS President Dragan P. Uskoković

### **2024 MRS-SERBIA** Award for a Lasting and Outstanding Contribution to Materials Science and Engineering

We are pleased to announce that the Laureate of the 2024 MRS-Serbia Award for a Lasting and Outstanding Contribution to Materials Science and Engineering is

#### Prof. Dr. Vladimir P. Torchilin



He is awarded for his achievements in the area of Pharmaceutical Biotechnology and Nanomedicine.

This is the decision of the MRS-Serbia Executive Board:

The Executive Board of the MRS-Serbia Presidency at their online meeting held on February 15<sup>th</sup>, 2024, considered the submitted nomination for the MRS-Serbia's 2024 Award for a Lasting and Outstanding Contribution to Materials Science and Engineering and concluded that the procedure was conducted in accordance with the Awarding Rulebook, that the Call was announced on the MRS-Serbia's website on December 31<sup>st</sup>, 2023, and that in the stipulated period of 45 days only one nomination was submitted.

Having received the opinion from the Expert Committee members: Prof. Dr. Dragan Uskoković (President of MRS-Serbia), Prof. Dr. Yury Gogotsi (Chair of YUCOMAT Conferences International Advisory Board and 2021 Laureate), Prof. Dr. Robert Sinclair (Honorary Chair of YUCOMAT Conferences International Advisory Board and 2021 Laureate), Prof. Dr. Robert Sinclair (Honorary Chair of YUCOMAT Conferences International Advisory Board and 2020 Laureate), Prof. Dr. Dejan Raković (Vice-President of MRS-Serbia), Prof. Dr. Slobodan Milonjić (President of the Council and Member of the Presidency of MRS-Serbia), Prof.Dr.Nenad Ignjatović (Member of the Presidency and Secretary General of MRS-Serbia) Prof. Dr. Ivan Božović (2015 Laureate), Prof. Dr. Gordana Vunjak-Novaković (2016 Laureate), Prof. Dr.Velimir Radmilović (2017 Laureate), Prof. Dr. László Forró (2018 Laureate) Prof. Danilo Suvorov (2019 Laureate), Prof. Dr. Richard W. Siegel (2022 Laureate) and Prof. Dr. Knut Urban (2023 Laureate), the Executive Board of the MRS-Serbia Presidency took the decision that Prof. Dr. Vladimir P. Torchilin should be granted MRS-Serbia's 2024 Award for a Lasting and Outstanding Contribution to Materials Science and Engineering.

Prof. Torchilin was strongly supported by Prof. Dr. Dragan Uskoković, Dr. Slobodan Milonjić, Prof. Dr. Velimir Radmilović, Prof. Dr. Dejan Raković, Prof. Dr. Nenad Ignjatović, Prof. Dr. Djordje Janaćković and Dr. Vuk Uskoković.

Prof. Torchilin's Honorary Plenary lecture will be presented during the Opening Ceremony of the 25<sup>th</sup> MRS-Serbia Annual Conference YUCOMAT 2024, starting at 9.00 am on Monday, September 2<sup>nd</sup>, 2024.

President of MRS-Serbia, Prof. Dr. Dragan Uskoković Vice-President of MRS-Serbia, Prof. Dr. Velimir Radmilović Vice-President of MRS-Serbia, Prof. Dr. Dejan Raković General Secretary of MRS-Serbia, Prof. Dr. Nenad Ignjatović

#### MATERIALS RESEARCH SOCIETY OF SERBIA

#### President of the

Council:Slobodan MilonjićPresident:Dragan UskokovićVice-presidents:Velimir Radmilović, Dejan Raković

Members:Gordana Ćirić-Marjanović, Vera Dondur, Đorđe Janaćković, Đuro Koruga,<br/>Slavko Mentus, Bojana Obradović, Zoran Petrović, Milenko Plavšić, Zoran<br/>Popović, Vladimir Srdić, Jovan Šetrajčić, Petar Uskoković, Miodrag<br/>Zlatanović

#### **International Advisory Board**

Honorary Chair: Robert Sinclair (USA)

Chair: Yury Gogotsi (USA)

Members: Pulickel Ajayan (USA), Markus Antonietti (Germany), Xavier Batlle (Spain), Yoshio Bando (China), David C.Bell (USA), Serena Best (UK), S. Jeffrey Brinker (USA), Ivan Božović (USA), Philippe Colomban (France), Uli Dahmen (USA), Rafal Dunin-Borkowski (Germany), Andrea C. Ferrari (UK), Mauro Ferrari (USA), Laszlo Forro (USA), Elvira Maria Correia Fortunato (Portugal), Hamis Fraser (USA), Aharon Gedanken (Israel), Patrick Gane (Finland), Horst Hahn (Germany), Robert Hull (USA), Lei Jiang (China), Prashant V. Kamath (USA), Jose M. Kenny (Italy), Alexander H. King (USA), Feng-Huei Lin (Taiwan), Arumugam Manthiram (USA), Milan Mrksich (USA), Mohammad Khaja Nazeeruddin (Switzerland), Eva Olsson (Sweden), Eiji Osawa (Japan), Davor Pavuna (Switzerland), Doug Perovic (Canada), Robert Ritchie (USA), John A. Rogers (USA), Peter Franz Rogl (Austria), Frances Ross (USA), Richard W. Siegel (USA), Mamoru Senna (Japan), Danilo Suvorov (Slovenia), Samuel I. Stupp (USA), Enrico Traversa (Italy), Vladimir Torchilin (USA), Shizhang Qiao (Australia), Knut Urban (Germany), Vuk Uskoković (USA), Ruslan Z, Valiev (Russia), Gordana Vunjak Novaković (USA), Paul Weiss (USA), Jackie Ying (Singapore), Dongyuan Zhao (China), Yuntian T. Zhu (Hong Kong, China)

The First Conference on materials science and engineering, including physics, physical chemistry, condensed matter chemistry, and technology in general, was held in September 1995, in Herceg Novi. An initiative to establish Yugoslav Materials Research Society was born at the conference and, similar to other MR societies in the world, the programme was made, and objectives determined. The Yugoslav Materials Research Society (Yu-MRS), a non-government and non-profit scientific association, was founded in 1997 to promote multidisciplinary goal-oriented research in materials science and engineering. Main task and objective of the Society is to encourage creativity in materials research and engineering to reach a harmonic coordination between achievements in this field in our country and analogous activities in the world with an aim to include our country into the global international projects. Until 2003, Conferences were held every second year and then they grew into Annual Conferences that were traditionally held in Herceg Novi in September of every year. Following the political separation between Serbia and Montenegro, in 2007 Yu-MRS formed two new MRS: MRS-Serbia (official successor of Yu-MRS) and MRS-Montenegro (in founding). In 2008 MRS-Serbia became a member of FEMS (Federation of European Materials Societies).

#### INTERNATIONAL INSTITUTE FOR THE SCIENCE OF SINTERING

Managing Board

President:	Prof. Danilo Suvorov
President of Managing Board	l: Prof. Dragan P. Uskoković
Members of Managing Board: Prof. Rajendra Bordia, Prof. Suk-Joong L. Kang, Prof. Bernd	
	Kieback, Prof. Zoran S. Nikolić, Prof. Eugen A. Olevsky, Prof.
	Andrey B. Ragulya, Prof. Masahiro Yoshimura
General secretary:	Prof. Biljana Stojanović
Conference Local (Serbia)	
Co-chair:	Prof. Biljana Stojanović, Prof. Đorđe Janaćković

The International Institute for the Science of Sintering (IISS https://www.iiss-sci.org) was originally established in 1968 as the International Team of Study of Sintering, based in Belgrade, Yugoslavia (today the Republic of Serbia) at the Vinča Institute of Nuclear Science. The founding assembly was held the next year in Herceg Novi, and it brought about one hundred scientists from different parts of the world. This was an open symposium where all the founders gave plenary lectures on their most up-to- date research. The team decided to organize this conference at the same place every other year. After the first one, the interest grew rapidly in the world, so by 1973 many new members joined. The International Team for the Study of Sintering soon became the International Institute for the Science of Sintering. At the initiative of the President of the Serbian Academy of Science and Arts (SASA). Pavle Savić. the Institute received the patronage of SASA and eminent institutions from the member countries. At that time, the Institute played an enormous role in bringing scientists from all over the world closer together. This was especially important during the Cold War when Yugoslavia was the only place where scientists from the East and from the West could meet. The 11th conference was held in 2019 in Herceg Novi, Montenegro (https://www.mrsserbia.org.rs/files/50.pdf) in the same hotel resort where the first conference was organized more than 50 years ago. It re-established the activity of the Institute and marked the new beginning of a new series of famous Yugoslav Sintering Conferences.

This is the third WRTCS Conference held together with YUCOMAT after 15 years of inactivity, following the decision of the Institute's Board of Directors to renew its work. Significant progress is already noticeable. New members have been elected, so now there are 93 actives, out of 183 elected so far. We have created a nice website where all information is timely updated. Year after year, the number of papers at WRTCS increases, and this year there will be about thirty, including 9 plenary lectures. Just before the Conference, from August 30 to September 1, three IISS members (Prof. Suk-Joong L. Kang - KAIST, Prof. Eugene A. Olevsky - San Diego State University, and Prof. Vincenzo Sglavo - University of Trento) held an 18-hour Tutorial for young researchers. The Managing Board's suggestion to start awarding Institute Prizes to encourage greater activity among members was honored, and after 22 years, it was decided to award the Frenkel Prize "for extraordinary contributions to the Science of Sintering" to two of our most distinguished and active members this year.

#### YUCOMAT 2024 & XIII WRTCS COMMITTEES

#### **Conference Organising Committee**

Chairpersons:	Đorđe Veljović, Zoran Jovanović
Members:	Branko Matović, Irena Nikolić, Bojana Obradović, Vuk Radmilović, Veljko Đokić, Ljiljana Damnjanović, Sonja Jovanović, Aleksandar Dekanski, Mira Vukčević, Željko Radovanović, Ivana Dinić, Milica Vujković

**Conference Secretary:** Jasmina R. Jevtić

#### **Conference Technical Committee:**

Željko Mravik, Jelena Rmuš Mravik, Milica Pejčić, Marija Grujičić, Tamara Matić, Vukašin Ugrinović, Jana Petrović, Nemanja Barać, Jelena Petrović, Ivana Banićević, Jovan Lukić, Srđan Perišić, Anđela Radisavljević, Daniel Mijailović, Jana Mišurović, Minea Kapidžić

#### **GENERAL INFORMATION**

DATE AND VENUE: The joint event YUCOMAT 2024 & XIII WRTCS conferences will be held on September 2 - 6, 2024, at the Hunguest Hotel Sun Resort, in Herceg Novi, Montenegro. Participants will also be accommodated there. The conference will begin on Monday, September 2<sup>nd</sup>, at 09.00 and end on Friday, September 6<sup>th</sup>, 2024, at 12.00.

REGISTRATION: Registration, registration fee payment, conference materials distribution, etc, will take place at the conference desk, open on: Sunday to Tuesday from 7.30 to 19.00, on Wednesday and Thursday from 8.00-12.00 and 19.00-20.00, and on Friday from 8.00 to 12.00. At registration, the participants are requested to submit proof of their advance registration fee payment to the Conference Secretariat.

INSTRUCTION FOR AUTHORS: The conference will feature Plenary Sessions, Oral Sessions, Poster Sessions. Time available for delivery is 40 min for Plenary Session and 15 min for Oral Session papers, including discussion. Video-beam is available. PowerPoint presentations, recorded on USB flash-memory, should be given at the start of the session. In Poster Sessions, the authors are requested to display their posters minimum one hour before the session and to be present beside their posters during the session. Poster sessions' venue will be open from Tuesday to Thursday.

CONFERENCE AWARDS: Award by MRS-Serbia at the YUCOMAT 2024 Conference to the authors not older than 35 for the best: Three Oral presentation and Three Posters presentation and best PhD completed between the two YUCOMAT conferences. Awarded authors will be announced at the Closing Ceremony of the Conference. Each award consists of diploma, meeting registration fee to attend the next YUCOMAT 2025 Conference, and a one-year MRS Serbia membership.

ADDITIONAL ACTIVITIES: Traditional Cocktail Party on Monday evening and excursion on Thursday afternoon (boat trip around Boka Kotorska Bay) will be organized again.

#### **GENERAL YUCOMAT 2024 & XIII WRTCS PROGRAM**

#### Sunday, September 1, 2024

08<sup>00</sup> - 19<sup>00</sup> **Registration** 

#### Monday, September 2, 2024

- 08<sup>00</sup> 19<sup>00</sup> **Registration**
- 09<sup>00</sup> 09<sup>45</sup> **OPENING CEREMONY**, Main Conference Hall
- 09<sup>45</sup> 10<sup>30</sup> The Laureate of the 2024 MRS-Serbia, Award for a Lasting and Outstanding Contribution to Materials Science and Engineering
- 11<sup>00</sup> 13<sup>00</sup> First YUCOMAT Plenary Session, Main Conference Hall
- 13<sup>15</sup> Photo Session
- 15<sup>00</sup> 17<sup>40</sup> First WRTCS Plenary Session, Main Conference Hall
- 19<sup>30</sup> 22<sup>00</sup> Cocktail Party

#### Tuesday, September 3, 2024

- 08<sup>00</sup> 09<sup>45</sup> **First YUCOMAT & WRTCS Poster Session**, National Restaurant Jadranka Terrace **Competition for the best Poster Presentation of young researchers**
- 10<sup>00</sup> 13<sup>20</sup> Second WRTCS Plenary Session, Main Conference Hall
- 15<sup>00</sup> 17<sup>45</sup> **First YUCOMAT Oral Session**, Main Conference Hall **Competition for the best oral presentation of young researchers**

#### Wednesday, September 4, 2024

- 08<sup>00</sup> 09<sup>45</sup> Second YUCOMAT & WRTCS Poster Session, National Restaurant Jadranka Terrace
- 10<sup>00</sup> 13<sup>00</sup> Second YUCOMAT Plenary Session, Main Conference Hall
- 15<sup>00</sup> 16<sup>30</sup> **First WRTCS Oral Session**, Main Conference Hall

#### Competition for the best oral presentation of young researchers

16<sup>30</sup> - 17<sup>30</sup> Second WRTCS Oral Session, Main Conference Hall

#### Thursday, September 5, 2024

- 08<sup>00</sup> 09<sup>45</sup> Third YUCOMAT Poster Session, National Restaurant Jadranka Terrace
- 10<sup>00</sup> 12<sup>40</sup> Third YUCOMAT Plenary Session, Main Conference Hall
- 14<sup>00</sup> 19<sup>00</sup> Boat-trip around Boka Kotorska Bay

#### Friday, September 6, 2024

- 09<sup>00</sup> 11<sup>45</sup> Second and Third YUCOMAT Oral Session, Main and Small Conference Hall
- 12<sup>00</sup> Awards and Closing of the Conference
- 12<sup>30</sup> Farewell Cocktail

#### SCIENTIFIC YUCOMAT 2024 & XIII WRTCS PROGRAM

Sunday, September 1, 2024

08<sup>00</sup> - 19<sup>00</sup> **Registration** 

#### Monday, September 2, 2024

- 08<sup>00</sup> 19<sup>00</sup> **Registration**
- 09<sup>00</sup> 10<sup>30</sup> **OPENING CEREMONY**, Main Conference Hall
- 09<sup>00</sup> 09<sup>45</sup> Welcome Speech **Dragan Uskoković**, president of MRS-Serbia Welcome Address - **Robert Sinclair**, Honorary Chair and **Yury Gogotsi**, *Chair of the International Advisory Board*

#### Awards of Appreciation for a Lasting and Outstanding Contribution to MRS-Serbia and IISS

**Presentation of YUCOMAT 2023 Awards** for young authors with the best PhD thesis, oral and poster presentations

09<sup>45</sup> - 10<sup>30</sup> MRS-Serbia 2024 Award for a Lasting and Outstanding Contribution to Materials Science and Engineering

Stimuli-sensitive drug delivery system

Vladimir Torchilin

Center for Pharmaceutical Biotechnology & Nanomedicine, Northeastern University, Boston, MA, USA

10<sup>30</sup> - 11<sup>00</sup> Break

First YUCOMAT Plenary Session, Main Conference Hall

Session: 11<sup>00</sup> - 13<sup>00</sup>

Chairpersons: Robert Sinclair, Yury Gogotsi and Andrey Rogach

- 11<sup>00</sup> 11<sup>40</sup> Y.PL.S.I.1
  - **TEM-STEM Studies of Gold Nanoparticles in Twisted MoS**<sub>2</sub> **Bilayers** <u>Robert Sinclair</u><sup>1</sup>, Yi Cui<sup>1</sup>, Pawel Czaja<sup>1,2</sup>, Yi Cui<sup>1</sup>

<sup>1</sup>Department of Materials Science and Engineering, Stanford University, Stanford, United States; <sup>2</sup>Institute of Metallurgy and Materials Science, Polish Academy of Sciences, Krakow, Poland

#### 11<sup>40</sup> - 12<sup>20</sup> Y.PL.S.I.2

#### Synthesis of MXenes by Selective Etching and Chemical Vapor Deposition (CVD) Yury Gogotsi

A.J. Drexel Nanomaterials Institute and Department of Materials Science and Engineering, Drexel University, Philadelphia, USA

#### 12<sup>20</sup> - 13<sup>00</sup> Y.PL.S.I.3

#### **Colloidal nanomaterials for light**

Andrey Rogach

Department of Materials Science and Engineering & Centre for FunctionalPhotonics, City University of Hong Kong, Hong Kong S.A.R.

- 13<sup>15</sup> Photo Session
- 13<sup>30</sup> 15<sup>00</sup> Break

First WRTCS Plenary Session, Main Conference Hall				
Session: 15 <sup>00</sup> - 17 <sup>40</sup>				
	ons: Eugene Olevsky, Suk-Joong L. Kang and Olivier Guillon			
15 <sup>00</sup> - 15 <sup>40</sup>				
	Sintering-Assisted Additive Manufacturing			
	Eugene Olevsky			
	College of Engineering, San Diego State University, USA			
15 <sup>40</sup> - 16 <sup>20</sup>	W.PL.S.I.2			
	What we understand and what we need to know in sintering			
	Suk-Joong L. Kang			
	KAIST, Daejeon, Republic of Korea			
16 <sup>20</sup> - 17 <sup>00</sup>	W.PL.S.I.3			
	Advanced sintering methods for solid-state batteries			
	<u>Olivier Guillon</u>			
	Institute of Energy and Climate Research: Materials Synthesis and Processing,			
	Forschungszentrum Jülich and RWTH Aachen University, Germany			
17 <sup>00</sup> - 17 <sup>40</sup>	W.PL.S.I.4			
	Non-isothermal sintering of nanostructured particulate materials: Dream			
	or reality?			
	Andrey V. Ragulya			
	Frantsevich Institute of Problems in Materials Science NAS of Ukraine, Kyiv, Ukraine			
19 <sup>30</sup> - 22 <sup>00</sup>	Cocktail Party			
	•			
Tuesday	y, <u>September 3, 2024</u>			
First YUCC	MAT & WRTSC Poster Session, National Restaurant Jadranka Terrace			
	on for the best Poster Presentation of young researchers			
Session: 08				
Chairpersons: Zoran Jovanović, Đorđe Veljović				
YUCOMAT SYMPOSIUM A:				
ADVANCED METHODS IN SYNTHESIS AND PROCESSING OF MATERIALS				
P.S.I.A.1	Influence of Common Catalysts on Curing Kinetics of Polyurethanes:			
	Non-isothermal Rheological Method			

<u>Mladen Timotijević</u><sup>1</sup>, Ivan Dimitrijević<sup>2</sup>, Danica Bajić<sup>1</sup> <sup>1</sup>Military Technical Institute, Belgrade, Serbia, <sup>2</sup>Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia

#### **P.S.I.A.2 Optomagnetic imaging spectroscopy in human kidney cancer detection** <u>Aleksandra Dinić</u><sup>1</sup>, Lidija Matija<sup>1</sup>, Branislava Jeftić<sup>1</sup>, Ivana Stanković<sup>1</sup>, Gorana Nikolić<sup>2</sup>

<sup>1</sup>Department of Biomedical Engineering, Faculty of Mechanical Engineering, University of Belgrade, Serbia, <sup>2</sup>Institute of Pathology, Faculty of Medicine, University of Belgrade, Serbia

#### P.S.I.A.3 Mechanochemical Synthesis of Ammonium-Iminodiacetato-Dithiocarbamate: An Environmentally Friendly Approach <u>Slađana Kovačević</u><sup>1</sup>, Milica Kosović Perutović<sup>1</sup>, Marija Ristić<sup>2</sup>, Jana Mišurović<sup>1</sup>, Zorica Leka<sup>1</sup> <sup>1</sup>University of Montenegro, Faculty of Metallurgy and Technology, , Podgorica,

<sup>1</sup>University of Montenegro, Faculty of Metallurgy and Technology, , Podgorica, Montenegro, <sup>2</sup>University of Kragujevac, Faculty of Science, Kragujevac, Serbia

### **P.S.I.A.4** Synthesis of highly porous Ti<sub>3</sub>AlC<sub>2</sub> MAX-phase resulting Ti<sub>3</sub>C<sub>2</sub> MXene with enhanced properties

<u>Veronika Zahorodna<sup>1,2</sup></u>, Ivan Baginskiy<sup>1</sup>, Serhii Dukhnovskyi<sup>1</sup>, Veronika Kaurkovska<sup>1</sup>, Margaryta Potashna<sup>1</sup>, Stefano Ippolito<sup>3</sup>, Oleksiy Gogotsi<sup>1,2</sup>, Iryna Roslyk<sup>1,3</sup>, Yury Gogotsi<sup>3</sup>

<sup>1</sup>Materials Research Centre Ltd., Kyiv, Ukraine, <sup>2</sup>Y-Carbon ltd. (Carbon-Ukraine), Kyiv, Ukraine, <sup>3</sup>Drexel University, Philadelphia, USA

#### YUCOMAT SYMPOSIUM B:

#### ADVANCED MATERIALS FOR HIGH-TECHNOLOGY APPLICATION

P.S.I.B.1 Role of Surface Terminations in MXene Thermodynamic Stability <u>Ervin Rems<sup>1,2</sup></u>, Yong-Jie Hu<sup>3</sup>, Yury Gogotsi<sup>3,4</sup>, Robert Dominko<sup>1,2</sup> <sup>1</sup>Department of Materials Chemistry, National Institute of Chemistry, Ljubljana, Slovenia, <sup>2</sup>Faculty of Chemistry and Chemical Technology, University of Ljubljana, Ljubljana, Slovenia, <sup>3</sup>Department of Materials Science and Engineering, Drexel University, Philadelphia, USA, <sup>4</sup>A.J. Drexel Nanomaterials Institute, Drexel University,

Philadelphia, USA

#### **P.S.I.B.2** Assessing the charge storage capability of hydrothermally treated biomassderived activated carbon in different electrolyte formulations

<u>Minea Kapidžić</u><sup>1</sup>, Jana Mišurović<sup>1</sup>, Veselinka Grudić<sup>1</sup>, Milica Vujković<sup>2,3</sup> <sup>1</sup>University of Montenegro, Faculty of Metallurgy and Technology, Podgorica, Montenegro, <sup>2</sup>University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia, <sup>3</sup>Center for Interdisciplinary and Multidisciplinary Studies, University of Montenegro, Podgorica, Montenegro

### **P.S.I.B.3** Exploring the potential of olive mill waste for the production of energy storage materials

<u>Kristina Lalatović</u><sup>1</sup>, Minea Kapidžić<sup>1</sup>, Sonja Kastratović<sup>1</sup>, Veselinka Grudić<sup>1</sup>, Milica Vujković<sup>2,3</sup>, Jana Mišurović<sup>1</sup>

<sup>1</sup>University of Montenegro, Faculty of Metallurgy and Technology, Podgorica, Montenegro, <sup>2</sup>University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia, <sup>3</sup>Center for Interdisciplinary and Multidisciplinary Studies, University of Montenegro, Podgorica, Montenegro

### **P.S.I.B.4** Ambient pressure RWGS reaction: Advancements in reactor design and catalyst efficiency

<u>Dimitrij Ješić</u>, Blaž Likozar National Institute of Chemistry, Ljubljana, Slovenia

#### YUCOMAT SYMPOSIUM C: NANOSTRUCTURED MATERIALS

### **P.S.I.C.1** Impact of molybdenum disulfide morphology on catalytic activity for hydrogen evolution reaction

<u>Jelena Rmuš Mravik</u><sup>1</sup>, Blaž Belec<sup>2</sup>, Milica Prvulović<sup>1</sup>, Bojana Babić<sup>1</sup>, Tijana Pantić<sup>1</sup>, Jasmina Grbović Novaković<sup>1</sup>, Sandra Kurko<sup>1</sup>

<sup>1</sup>Center of excellence for hydrogen and renewable energy, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia; <sup>2</sup>Materials Research Laboratory, University of Nova Gorica, Ajdovščina, Slovenia

**P.S.I.C.2** Correlation between photoluminescence and photocatalytic properties of novel down and up-converting phosphors

<u>Tijana Stamenković</u>, Vesna Lojpur

Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Vinča, Belgrade, Serbia

**P.S.I.C.3** The magnetic properties of CoFe<sub>2</sub>O<sub>4</sub> and CoFe<sub>2</sub>O<sub>4</sub>/SiO<sub>2</sub> prepared by thermal decomposition method

<u>Ljubica Andjelković</u><sup>1</sup>, Marija Šuljagić<sup>1</sup>, Ana Mraković<sup>2</sup>, Vladimir Pavlović<sup>3</sup>, Marin Tadić<sup>2</sup>

<sup>1</sup>University of Belgrade - Institute of Chemistry, Technology and Metallurgy, Department of Chemistry, Belgrade, Serbia, <sup>2</sup>"VINČA" Institute of Nuclear Sciences -National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia, <sup>3</sup>University of Belgrade, Faculty of Agriculture, Belgrade, Serbia

### **P.S.I.C.4** Surface chemistry of hydrothermally treated GO and GO-based nanocomposites

<u>Milica Pejčić<sup>1</sup></u>, Željko Mravik<sup>1</sup>, Danica Bajuk-Bogdanović<sup>2</sup>, Marija Grujičić<sup>1</sup>, Darija Petković<sup>1</sup>, Janez Kovač<sup>3</sup>, Zoran Jovanović<sup>1</sup>

<sup>1</sup>Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia, <sup>2</sup>Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia, <sup>3</sup>Department of Surface Engineering and Optoelectronics, Jožef Stefan Institute, Ljubljana, Slovenia

### **P.S.I.C.5** Modified glassy carbon electrodes with Zn/Ga-substituted cobalt ferrite for electrochemical detection of gallic acid

<u>Marija Grujičić</u><sup>1</sup>, Milica Pejčić<sup>1</sup>, Danica Bajuk-Bogdanović<sup>2</sup>, Marko Jelić<sup>1</sup>, Zoran Jovanović<sup>1</sup>, Ivana Stojković Simatović<sup>2</sup>, Sonja Jovanović<sup>1</sup> <sup>1</sup>Laboratory of Physics, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia, <sup>2</sup>Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia

### **P.S.I.C.6** Structural and magnetic properties of nanometric ε-Fe<sub>2</sub>O<sub>3</sub> prepared by microemulsion method

<u>Marija Šuljagić</u><sup>1</sup>, Ljubica Andjelković<sup>1</sup>, Ana Mraković<sup>2</sup>, Vladimir Pavlović<sup>3</sup>, Marin Tadić<sup>2</sup>

<sup>1</sup>University of Belgrade - Institute of Chemistry, Technology and Metallurgy, Department of Chemistry, Njegoševa 12, Belgrade, Serbia, <sup>2</sup>"VINČA" Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia, <sup>3</sup>University of Belgrade, Faculty of Agriculture, Zemun -Belgrade, Serbia

#### YUCOMAT SYMPOSIUM D: ECO-MATERIALS AND ECO-TECHNOLOGIES

**P.S.I.D.1** Surfactant-modified bentonites for the removal of nonsteroidal antiinflamatory drug: targeting ibuprofen

<u>Danijela Smiljanić</u><sup>1</sup>, Aleksandra Daković<sup>1</sup>, Milena Obradović<sup>1</sup>, Milica Ožegović<sup>1</sup>, Marija Marković<sup>1</sup>, Milica Todorović<sup>2</sup>

<sup>1</sup>Institute for Technology of Nuclear and Other Mineral Raw Materials, Belgrade, Serbia, <sup>2</sup>University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia

P.S.I.D.2	<b>Solid residue of pyrolysis of agricultural waste as an alternative fossil fuel</b> Emilija N. Vukićević <sup>1</sup> , Jelena N. Isailović <sup>2</sup> , Gordana Gajica <sup>3</sup> , Vesna Antić <sup>2</sup> , Mališa Antić <sup>2</sup> , Jan Schwarzbauer <sup>4</sup> , <u>Branimir Jovančićević<sup>1</sup></u> <sup>1</sup> University of Belgrade, Faculty of Chemistry, Serbia, <sup>2</sup> University of Belgrade, Faculty of Agriculture, Zemun, Belgrade, Serbia, <sup>3</sup> University of Belgrade, Institute of Chemistry Technology and Metallurgy (IChTM), Belgrade, Serbia, <sup>4</sup> RWTH Aachen University,
	Aachen, Germany

P.S.I.D.3 Investigation of various catalytic materials for heterogeneous conversion of biomass-derived glycolic acid <u>Aleksa Kojčinović</u><sup>1</sup>, Florian Harth<sup>1,2</sup>, Blaž Likozar<sup>1</sup>, Miha Grilc<sup>1</sup> <sup>1</sup>Department of Catalysis and Chemical Reaction Engineering, National Institute of Chemistry, Ljubljana, Slovenia, <sup>2</sup>Institute of Chemical Technology, Universiät Leipzig, Leipzig, Germany

#### YUCOMAT SYMPOSIUM E: BIOMATERIALS

- P.S.I.E.1 New approach of thin MXene coating for PCL membrane Yevheniia Husak<sup>1,2</sup>, Yuliia Varava<sup>1,2</sup>, Natalia Waloszczyk<sup>2</sup>, Viktoriia Korniienko<sup>1,3</sup>, Kateryna Diedkova<sup>1,3</sup>, Volodymyr Deineka<sup>1,3</sup>, Veronika Zahorodna<sup>4</sup>, Oleksiy Gogotsi<sup>4</sup>, Wojciech Simka<sup>2</sup>, Maksym Pogorielov<sup>1,3</sup> <sup>1</sup>Sumy State University, Sumy, Ukraine, <sup>2</sup>Silesian University of Technology, Gliwice,
- Poland, <sup>3</sup>University of Latvia, Riga, Latvia, <sup>4</sup>Materials Research Center Ltd, Kyiv, Ukraine
  P.S.I.E.2 MXene-based antifungal photothermal ablation Valeriia Korniienko<sup>1</sup>, Yuliia Varava<sup>1</sup>, Veronika Zahorodna<sup>3</sup>, Oleksiy Gogotsi<sup>3</sup>, Viktoriia Korniienko<sup>1,2</sup>, Maksym Pogorielov<sup>1,2</sup>
   <sup>1</sup>Sumy State University, Sumy, Ukraine; <sup>2</sup>University of Latvia, Riga, Latvia, <sup>3</sup>CARBON-UKRAINE Ltd., Kiev, Ukraine

#### WRTCS

**P.S.I.W.1** Synthesis and characterization of In-doped BaSnO<sub>3</sub> electrolyte for intermediate-temperature solid oxide fuel cells

<u>Jelena Mitrović</u><sup>1</sup>, Milica Počuča-Nešić<sup>1</sup>, Matejka Podlogar<sup>2</sup>, Aleksandar Malešević<sup>1</sup>, Aleksandar Radojković<sup>1</sup>, Olivera Zemljak<sup>1</sup>, Katarina Vojisavljević<sup>1</sup>, Zorica Branković<sup>1</sup>, Goran Branković<sup>1</sup>

<sup>1</sup>University of Belgrade, Institute for Multidisciplinary Research, Belgrade, Serbia, <sup>2</sup>Jožef Stefan Institute, Department for Nanostructured Materials, Ljubljana Slovenia

P.S.I.W.2 Comparison of TiCN-based cermets sintered under different atmospheres <u>René M. Guillen Pineda</u>, Hortensia Melero, Olivier Ther *Hyperion Materials & Technologies Spain, S.L.* 

P.S.I.W.3 Structural, microstructural and multiferroic properties of YMnO<sub>3</sub> ceramics co-doped with titanium and rare-earth metals <u>Olivera Zemljak</u><sup>1</sup>, Danijela Luković Golić<sup>1</sup>, Bojana Simović<sup>1</sup>, Pavla Šenjug<sup>2</sup>, Damir Pajić<sup>2</sup>, Matejka Podlogar<sup>3</sup>, Aleksandar Malešević<sup>1</sup>, Jelena Mitrović<sup>1</sup>, Goran Branković<sup>1</sup>, Zorica Branković<sup>1</sup> <sup>1</sup>Institute for Multidisciplinary Research, University of Belgrade, Belgrade, Serbia, <sup>2</sup>Department of Physics, Faculty of Science, University of Zagreb, Zagreb, Croatia, <sup>3</sup>Department for Nanostructural Materials, Jožef Stefan Institute, Ljubljana, Slovenia

P.S.I.W.4	Application of powder metallurgy in the production of the copper-based material <u>Marko Simić</u> , Emilija Nidžović, Vladimir Pavkov, Jelena Stašić, Jovana Ružić	
	Department of Materials, "Vinča" Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia	
	Second WRTCS Plenary Session, Main Conference Hall Session: 10 <sup>00</sup> - 13 <sup>20</sup>	
Chairperso	ons: Jing-Feng Li and Ralf Riedel	
10 <sup>00</sup> - 10 <sup>40</sup>	W.PL.S.II.5	
	Spark plasma sintering of thermoelectric materials Jing-Feng Li	
1040 1120	School of Materials Science and Engineering, Tsinghua University, Beijing, China W.PL.S.II.6	
10 - 11	Flash sintering of carbides and borides	
	Vincenzo M. Sglavo, Emanuele De Bona, Isacco Mazo	
	Department of Industrial Engineering, University of Trento, Trento, Italy	
11 <sup>20</sup> - 12 <sup>00</sup>	W.PL.S.II.7	
	Synthesis and sintering of sulfide-based optical ceramics	
	<u>Yiquan Wu</u>	
	Kazuo Inamori School of Engineering, New York State College of Ceramics, Alfred	
	University, Alfred, New York, United States	
12 <sup>00</sup> - 12 <sup>40</sup>	W.PL.S.II.8	
	Powder-Free Processing of Advanced Ceramics with Multifunctional	
	Properties	
	Ralf Riedel	
12 <sup>40</sup> - 13 <sup>20</sup>	Institute of Materials Science, Darmstadt University of Technology, Darmstadt, Germany W.PL.S.II.9	
	Optimizing the performance of metastable beta titanium alloys through processing ( <i>e.g.</i> additive manufacturing) and heat-treatment	
	<u>Hamish L. Fraser</u>	
	Dept. of Materials Science and Engineering, The Ohio State University, Columbus, OH, USA	
13 <sup>20</sup> - 15 <sup>00</sup>	Break	
First YUCC	OMAT Oral Session, Main Conference Hall	
Competitie Session: 1	on for the best oral presentation of young researchers	
	ons: Bojana Obradović, Snežana Lazić	
YUCOMAT SYMPOSIUM B: ADVANCED MATERIALS FOR HIGH-TECHNOLOGY APPLICATION		
15 <sup>00</sup> - 15 <sup>15</sup> O.S.I.B.1		
	Halogen Bonding: A Pathway to More Stable Perovskite Solar Cells	

Jovan Lukić<sup>1,2</sup>, Vuk V. Radmilović<sup>1</sup>, Jovana V. Milić<sup>2</sup> <sup>1</sup>Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia, <sup>2</sup>Adolphe Merkle Institute, University of Fribourg, Fribourg, Switzerland

#### 15<sup>15</sup> - 15<sup>30</sup> **O.S.I.B.2**

#### Enhancing water splitting efficiency through structural and chemical modifications of cellulose-derived electrocatalysts based on nickel phosphides Klaudia Maślana, Karolina Pietrusewicz, Ewa Mijowska

West Pomeranian University of Technology, Szczecin, Faculty of Chemical Technology and Engineering, Department of Nanomaterials Physicochemistry, Szczecin, Poland

#### 15<sup>30</sup> - 15<sup>45</sup> **O.S.I.B.3**

#### **Cost-Efficient Method for Deterministic Creation of Single Photon Emitters in GaSe**

Sanja Djurdjić Mijin<sup>1,2</sup>, Ismael dePedro-Embid<sup>3</sup>, Snežana Lazić<sup>1,4,5</sup> <sup>1</sup>Departamento de Fisica de Materiales, Facultad de Ciencias, Universidad Autonoma de Madrid (UAM), Madrid, Spain, <sup>2</sup>Institute of Physics Belgrade, University of Belgrade, Belgrade, Serbia, <sup>3</sup>Paul-Drude-Institut fur Festkorperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany, <sup>4</sup>Instituto Universitario de Ciencia de Materiales "Nicolas Cabrera" (INC), UAM, Madrid, Spain, <sup>5</sup>Condensed Matter Physics Center (IFIMAC), UAM, Madrid, Spain

#### YUCOMAT SYMPOSIUM C: NANOSTRUCTURED MATERIALS

#### 15<sup>45</sup> - 16<sup>00</sup> **O.S.I.C.1**

**Progress in Bubble-Printing: Fabrication of Ti<sub>3</sub>C<sub>2</sub>TX MXene Strain Sensors** <u>Marcel Herber<sup>1,2</sup></u>, Eric H. Hill<sup>1,2</sup>

<sup>1</sup>Institute of Physical Chemistry, University of Hamburg, Hamburg, Germany, <sup>2</sup>The Hamburg Center for Ultrafast Imaging (CUI), Hamburg, Germany

#### 16<sup>00</sup> - 16<sup>15</sup> **O.S.I.C.2**

#### TM<sub>1/3</sub>TaS<sub>2</sub>-based Transition Metal Compound Catalysts: Driving Forward Scalable Alkaline Hydrogen Production via Bifunctional Electrocatalysis Levna Chacko. Sofer Zdeněk

Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Czech Republic

#### 16<sup>15</sup> - 16<sup>30</sup> **O.S.I.C.3**

### The impact of impurities on unconventional annealing of nanostructured copper

Michael Kerber<sup>1</sup>, Przemysław Suchecki<sup>2</sup>, Krzystof Sielicki<sup>2</sup>, Malgorzata Lewandowska<sup>2</sup>, Daria Setman<sup>1</sup>, <u>Agnieszka Krawczynska<sup>2</sup></u> <sup>1</sup>Faculty of Physics, University of Vienna, Vienna, Austria, <sup>2</sup>Faculty of Materials

Science and Engineering, Warsaw University of Technology, Warsaw, Poland

### YUCOMAT SYMPOSIUM D: ECO-MATERIALS AND ECO-TECHNOLOGIES 16<sup>30</sup> - 16<sup>45</sup> O.S.I.D.1

### Regulation of surface properties and structural defects of graphitic carbon nitride via oxygen doping and plasma treatment

Jana Petrović<sup>1</sup>, Željko Radovanović<sup>1</sup>, Bratislav Obradović<sup>2</sup>, Đorđe Janaćković<sup>3</sup>, Rada Petrović<sup>3</sup>

<sup>1</sup>Innovation Center of the Faculty of Technology and Metallurgy, Ltd, Belgrade, Serbia, <sup>2</sup>University of Belgrade, Faculty of Physics, Belgrade, Serbia, <sup>3</sup>University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia

#### YUCOMAT SYMPOSIUM E: BIOMATERIALS

#### 1645 - 1700 **O.S.I.E.1**

#### Perfusion-based 3D in vitro cell culture model for osteosarcoma cells: Biological and chemical engineering perspectives

<u>Ivana Banićević</u><sup>1</sup>, Mia Milošević<sup>1,2</sup>, Jelena Petrović<sup>1,2</sup>, Milena Milivojević<sup>3</sup>, Radmila Janković<sup>4</sup>, Jasmina Stojkovska<sup>1</sup>, Bojana Obradović<sup>1</sup>

<sup>1</sup>University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia, <sup>2</sup>Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia, <sup>3</sup>University of Belgrade, Institute of Molecular Genetics and Genetic Engineering, Belgrade, Serbia, <sup>4</sup>University of Belgrade, Faculty of Medicine, Belgrade, Serbia

#### 17<sup>00</sup> - 17<sup>15</sup> O.S.I.E.2

#### Size Matters: Exploring MXene-Cell Interactions

<u>Kateryna Diedkova<sup>1,2</sup></u>, Ena Enia<sup>1</sup>, Lita Grine<sup>1</sup>, Volodymyr Deineka<sup>1</sup>, Mārtiņš Borodušķis<sup>1</sup>, Ivan Baginskiy<sup>3</sup>, Veronika Zahorodna<sup>3</sup>, Oleksiy Gogotsi<sup>3</sup>, Maksym Pogorielov<sup>1,2</sup>

<sup>1</sup>Sumy State University, Sumy, Ukraine; <sup>2</sup>University of Latvia, Riga, Latvia; <sup>3</sup>Materials Research Center LTD, Kyiv, Ukraine

#### 17<sup>15</sup> - 17<sup>30</sup> **O.S.I.E.3**

### Thermodynamic characteristics of intermolecular interactions in the model bacterial membranes exposed to the LL-37 peptide action

<u>Katarzyna Pastuszak</u><sup>1</sup>, Małgorzata Jurak<sup>1</sup>, Marta Palusińska-Szysz<sup>2</sup> <sup>1</sup>Department of Interfacial Phenomena, Institute of Chemical Sciences, Faculty of Chemistry, Maria Curie-Skłodowska University, Lublin, Poland, <sup>2</sup>Department of Genetics and Microbiology, Institute of Biological Sciences, Faculty of Biology and Biotechnology, Maria Curie-Skłodowska University, Lublin, Poland

#### 17<sup>30</sup> - 17<sup>45</sup> **O.S.I.E.4**

### Alginate microfibers with incorporated hydroxyapatite particles for 3D osteosarcoma cell cultures and rapid anticancer drug screening

<u>Jelena Petrović<sup>1,2</sup></u>, Luka Bojić<sup>3</sup>, Milena Milivojević<sup>3</sup>, Ivana Banićević<sup>1</sup>, Radmila Janković<sup>4</sup>, Bojana Obradović<sup>1</sup>, Jasmina Stojkovska<sup>1</sup>

<sup>1</sup>University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia, <sup>2</sup>Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia, <sup>3</sup>University of Belgrade, Institute of Molecular Genetics and Genetic Engineering, Belgrade, Serbia, <sup>4</sup>University of Belgrade, Faculty of Medicine, Belgrade, Serbia

#### Wednesday, September 4, 2024

Second YUCOMAT & SINTERING Poster Session; National Restaurant Jadranka Terrace; Session: 08<sup>00</sup> - 09<sup>45</sup>

Chairpersons: Milica Vujković, Veljko Đokić

YUCOMAT SYMPOSIUM A:

#### ADVANCED METHODS IN SYNTHESIS AND PROCESSING OF MATERIALS

### P.S.II.A.5 Immobilization of yeast cells in biopolymer systems using freeze-drying technique

<u>Nataša Obradović</u><sup>1</sup>, Bojana Balanč<sup>2</sup>, Vukašin Ugrinović<sup>2</sup>, Verica Đorđević<sup>1</sup>, Nemanja Stanisavljević<sup>3</sup>, Mina Volić<sup>2</sup>, Viktor Nedović<sup>4</sup>

<sup>1</sup>University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia, <sup>2</sup>University of Belgrade, Innovation Center of Faculty of Technology and Metallurgy, Belgrade, Serbia,<sup>3</sup>University of Belgrade, Institute of Molecular Genetics and Genetic Engineering, Belgrade, Serbia, <sup>4</sup>University of Belgrade, Faculty of Agriculture, Zemun - Beograd, Serbia

### **P.S.II.A.6** In situ incorporation and calcination of Zn-Al LDH during PEO processing in close to neutral pH electrolytes

<u>Kristina Mojsilović</u><sup>1</sup>, Maria Serdechnova<sup>2</sup>, Carsten Blawert<sup>2</sup>, Mikhail L. Zheludkevich<sup>2,3</sup>, Stevan Stojadinović<sup>1</sup>, Rastko Vasilić<sup>1</sup>

<sup>1</sup>University of Belgrade, Faculty of Physics, Belgrade, Serbia, <sup>2</sup>Institute of Surface Science, Helmholtz-Zentrum Hereon, Geesthacht, Germany, <sup>3</sup>Institute of Materials Science, Faculty of Engineering, Kiel University, Kiel, Germany

### **P.S.II.A.7** Crack growth and deformation monitoring in additively manufactured pipe ring specimens using contactless measurement

<u>Isaak D. Trajković</u><sup>1</sup>, Miloš S. Milošević<sup>1</sup>, Aleksandar S. Sedmak<sup>2</sup>, Zoran M. Radosavljević<sup>3</sup>, Bojan I. Međo<sup>4</sup>

<sup>1</sup>Innovation center of the Faculty of Mechanical Engineering in Belgrade, Belgrade, Serbia, <sup>2</sup>University of Belgrade, Faculty of Mechanical Engineering, Belgrade, Serbia, <sup>3</sup>Research and Development Institute Lola, Belgrade, Serbia, <sup>4</sup>University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia

#### YUCOMAT SYMPOSIUM B:

#### ADVANCED MATERIALS FOR HIGH-TECHNOLOGY APPLICATION

P.S.II.B.5 Measurement Techniques for Dissolution of Solid Metal in Liquid Metal

<u>Krzysztof Kania<sup>1</sup></u>, Grzegorz Zając<sup>1</sup>, Jan Kudláček<sup>2</sup>, Dariusz Buchczik<sup>1</sup>, Jiří *Kuchai*<sup>2</sup>, *Franciszek Berger*<sup>3</sup>

<sup>1</sup>Silesian University of Technology, Faculty of Automatic Control, Electronics and Computer Science, Gliwice, Poland, <sup>2</sup>Czech Technical University, Faculty of Mechanical Engineering, Prague, Czech Republic, <sup>3</sup>Rockwell Automation sp. z o.o, Warszawa, Poland

### **P.S.II.B.6** Prediction and synthesis of low-work-function graphene nanostructures intercalated by alkali metals

<u>Yevhen Len<sup>1,2</sup></u>, Mykhailo Varvarin<sup>1,2</sup>, Vitalii Lebed<sup>1,2</sup>, Oleh Feia<sup>1,2</sup>, Oksana Lisova<sup>1,3</sup>, Iryna Galstian<sup>1</sup>

<sup>1</sup>G.V. Kurdyumov Institute for Metal Physics of NASU, Kyiv, Ukraine, <sup>2</sup>Kyiv Academic University, Kyiv, Ukraine, <sup>3</sup>Chuiko Institute of Surface Chemistry of NASU, Kyiv, Ukraine

- P.S.II.B.7 Kinetics of positive ions in H<sub>2</sub> gas <u>Željka Nikitović</u>, Zoran Raspopović Institute of Physics University of Belgrade, Belgrade, Serbia
- P.S.II.B.8 Adsorption-desorption processes on polymer-carbon coatings for solar energy collectors Mykola Sheychenko, Iryna Calstian, Yulia Bozhey, Mykhailo Bud, Eygen Le

Mykola Shevchenko, <u>Iryna Galstian</u>, Yulia Bozbey, Mykhailo Rud, Evgen Len G.V. Kurdyumov Institute for Metal Physics, N.A.S. of Ukraine, Kyiv, Ukraine

- P.S.II.B.9 Zn-species containing oxide coatings: photocatalysts vs. adsorption <u>Nenad Tadić</u><sup>1</sup>, Kristina Mojsilović<sup>1</sup>, Srna Stojanović<sup>2</sup>, Ljiljana Damjanović-Vasilić<sup>2</sup>, Stevan Stojadinović<sup>1</sup>, Rastko Vasilić<sup>1</sup> <sup>1</sup>University of Belgrade, Faculty of Physics, Belgrade, Serbia, <sup>2</sup>University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia
- P.S.II.B.10 Impact of the hybrid graphene-dielectric metasurface resonant oscillations on the propagation properties of surface plasmon-polaritons using simulation techniques

<u>Zoya E. Eremenko,</u>

Usykov Institute for Radiophysics and Electronics NASU, Kharkiv, Ukraine

P.S.II.B.11 CFD study of magnetic hysteresis heating in monolith reactor Andraž Pavlišič<sup>1</sup>, Anja Sedminek<sup>2</sup>, Sašo Gvergyek<sup>2</sup>

<sup>1</sup>National Institute of Chemistry, Ljubljana, Slovenia, <sup>2</sup>Jozef Stefan Institute, Ljubljana, Slovenia

#### YUCOMAT SYMPOSIUM C: NANOSTRUCTURED MATERIALS

P.S.II.C.7 High-Entropy Oxides: A New Frontier in Photocatalytic CO<sub>2</sub> Hydrogenation <u>Igor Djerdj<sup>1</sup></u>, Dalibor Tatar<sup>1</sup>, Habib Ullah<sup>2</sup>, Mohit Yadav<sup>3</sup>, Jelena Kojčinović<sup>1</sup>, Stjepan Šarić<sup>1</sup>, Imre Szenti<sup>3</sup>, Tina Skalar<sup>4</sup>, Matjaž Finšgar<sup>5</sup>, Mi Tian<sup>2</sup>, Ákos Kukovecz<sup>3</sup>, Zoltán Kónya<sup>3</sup>, András Sápi<sup>3</sup>

<sup>1</sup>Department of Chemistry, Josip Juraj Strossmayer University of Osijek, Osijek, Croatia, <sup>2</sup>Department of Engineering, Faculty of Environment, Science and Economy, University of Exeter, Penryn Campus, Cornwall, United Kingdom, <sup>3</sup>Department of Applied and Environmental Chemistry, University of Szeged, Szeged, Hungary, <sup>4</sup>Faculty of Chemistry and Chemical Technology, University of Ljubljana, Ljubljana, Slovenia, <sup>5</sup>Faculty of Chemistry and Chemical Engineering, University of Maribor, Maribor, Slovenia

**P.S.II.C.8** State diagrams of systems based on iron oxide and REE as a basis for creating magnetic materials

<u>Olga Chudinovych<sup>1,2</sup></u>, Olena Olifan<sup>1</sup>

<sup>1</sup>Frantsevich Institute for Problems of Materials Science of the NAS of Ukraine, Kyiv, Ukraine, <sup>2</sup>National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Kyiv, Ukraine

### **P.S.II.C.9** Graphene oxide-based nanocomposites on interdigital electrodes for sensing applications

<u>Željko Mravik</u><sup>1</sup>, Milica Pejčić<sup>2</sup>, Marija Grujičić<sup>2</sup>, Jelena Rmuš Mravik<sup>1</sup>, Predrag Stolić<sup>3</sup>, Sonja Jovanović<sup>2</sup>, Zoran Jovanović<sup>1</sup>

<sup>1</sup>Center of Excellence for Hydrogen and Renewable Energy (CONVINCE), Laboratory of Physics, Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia, <sup>2</sup>Laboratory of Physics, Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia, <sup>3</sup>Technical faculty in Bor, University of Belgrade, Serbia, Bor

#### P.S.II.C.10 Synthesis of a hybrid core-shell nanoparticles for efficient photocatalysis under sunlight

Ivana Dinić<sup>1</sup>, Marina Vuković<sup>1</sup>, Bojan Marinković<sup>2</sup>, Paula Jardim<sup>3</sup>, Lidija Mančić<sup>1</sup> <sup>1</sup>Institute of Technical Science of SASA, Belgrade, Serbia, <sup>2</sup>Department of Chemical and Materials Engineering, Pontifical Catholic University of Rio de Janeiro Rio de Janeiro, Brazil, <sup>3</sup>Department of Metallurgical and Materials Engineering, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil

#### **P.S.II.C.11** Phonon Contribution in the Heat Conductivity of Some Typical Models of Crystalline Nanostructures

Jovan P. Šetrajčić<sup>1</sup>, Dušan I. Ilić<sup>2</sup>

<sup>1</sup>Academy of Sciences and Arts of the Republic of Srpska, Banja Luka, Republic of Srpska - Bosnia and Herzegovina, <sup>2</sup>University of Novi Sad, Faculty of Technical Sciences, Novi Sad, Vojvodina, Serbia

## P.S.II.C.12 Influence of synthesis conditions of ZIF-67/polyaniline 5-sulfosalicylate composites on the properties and electrochemical behaviour of their carbonization derivatives

Maja Ranković<sup>1</sup>, <u>Aleksandra Janošević Ležaić<sup>2</sup></u>, Marjetka Savić<sup>3</sup>, Nemanja Gavrilov<sup>1</sup>, Danica Bajuk-Bogdanović<sup>1</sup>, Igor Pašti<sup>1</sup>, Gordana Ćirić-Marjanović<sup>1</sup> <sup>1</sup>University of Belgrade- Faculty of Physical Chemistry, Belgrade, Serbia, <sup>2</sup>University of Belgrade-Faculty of Pharmacy, Belgrade, Belgrade, <sup>3</sup>Vinča Institute of Nuclear Science, University of Belgrade, National Institute of the Republic of Serbia, Belgrade, Serbia

#### P.S.II.C.13 Photocatalytic properties of Mo, W and Cu-doped bismuth vanadate Marko Jelić<sup>1</sup>, Danica Bajuk-Bogdanović<sup>2</sup>, Igor Pašti<sup>2</sup>, Jelena Erčić<sup>1</sup>, Zoran Jovanović<sup>1</sup>, <u>Sonja Jovanović<sup>1</sup></u>

<sup>1</sup>Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Serbia, <sup>2</sup>Faculty of Physical Chemistry, University of Belgrade, Serbia

#### YUCOMAT SYMPOSIUM D: ECO-MATERIALS AND ECO-TECHNOLOGIES

P.S.II.D.4 Tesla inspired quantum-holographic non-local epigenetic clue for improving integrative medicine & transpersonal psychology Dejan Raković University of Belgrade, Faculty of Electrical Engineering, Belgrade, Serbia

P.S.II.D.5 Co-ZSM5 and CoNi-ZSM5 zeolites for ORR in alkaline media <u>Jadranka Milikić</u><sup>1</sup>, Srna Stojanović<sup>1</sup>, Katarina Rondović<sup>1</sup>, Ljiljana Damjanović-Vasilić<sup>1</sup>, Vladislav Rac<sup>2</sup>, Kristina Radinović<sup>1</sup>, Biljana Šljukić<sup>1,3</sup> <sup>1</sup>University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia, <sup>2</sup>University of Belgrade, Faculty of Agriculture, Belgrade, Serbia, <sup>3</sup>Center of Physics and Engineering of Advanced Materials, Laboratory for Physics of Materials and Emerging Technologies, Instituto Superior Técnico, Universidade de Lisboa, Lisbon, Portugal

#### P.S.II.D.6 Incorporation of natural pyrophyllite into wood polymer composites <u>Srđan Perišić</u><sup>1</sup>, Anđela Radisavljević<sup>1</sup>, Aleksandar Grujić<sup>2</sup>, Jasna Stajić-Trošić<sup>2</sup>, Vesna Radojević<sup>3</sup>

<sup>1</sup>University of Belgrade, Innovation Centre of the Faculty of Technology and Metallurgy, Belgrade, Serbia, <sup>2</sup>University of Belgrade, Institute of Chemistry, Technology and Metallurgy, National Institute of the Republic of Serbia, Belgrade, Serbia, <sup>3</sup>University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia

#### YUCOMAT SYMPOSIUM E: BIOMATERIALS

#### P.S.II.E.3 Novel biocomposites based on activated charcoal and probiotics -ProHealingAC project

<u>Vesna Lazić</u><sup>1</sup>, Tanja Krunić<sup>2</sup>, Sonja Mojsilović<sup>3</sup>, Miloš Đuknić<sup>4</sup>, Andrea Osmokrović<sup>5</sup>

<sup>1</sup>University of Belgrade, Faculty of Agriculture, Belgrade, Serbia, <sup>2</sup>University of Belgrade, Innovation Center, Faculty of Technology and Metallurgy, Belgrade, Serbia, <sup>3</sup>University of Belgrade, Institute for Medical Research, Belgrade, Serbia, <sup>4</sup>University of Belgrade, Faculty of Medicine (School of Medicine), Belgrade, Serbia, <sup>5</sup>University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia

P.S.II.E.4 Study of copper-doped hydroxyapatite and copper-doped silicatesubstituted nanohydroxyapatite as antibacterial and antifungal materials <u>Nataliia Dmytrivna Pinchuk<sup>1,2</sup></u>, Agata Piecuch<sup>3</sup>, Sara Targońska<sup>2,4</sup>, Paulina Sobierajska<sup>2</sup>, Katarzyna Szyszka<sup>2</sup>, Oleksii Bezkrovnyi<sup>2</sup>, Rafał Ogórek<sup>3</sup>, Rafal Jakub Wiglusz<sup>2,5</sup> <sup>1</sup>Department of Functional Materials for Medical Application, Frantsevich Institute for Problems of Materials Science of the NAS of Ukraine, Kyiv, Ukraine, <sup>2</sup>Division of Biomedical Physicochemistry, Institute of Low Temperature and Structure Research Polish Academy of Sciences, Wrocław, Poland, <sup>3</sup>Department of Mycology and Genetics, Institute of Genetics and Microbiology, University of Wroclaw, Wroclaw, Poland, <sup>4</sup>Department of Molecular Sciences, Swedish University of Agricultural Sciences, Uppsala, Sweden, <sup>5</sup>Department of Organic Chemistry, Bioorganic Chemistry and Biotechnology, Silesian University of Technology, Gliwice, Poland

P.S.II.E.5 Antibacterial electrospun poly(ε-caprolactone) nanofiber mats loaded with cefazolin and meropenem for wound healing <u>Anđela Radisavljević</u><sup>1</sup>, Jasmina Stojkovska<sup>2</sup>, Ivan Jančić<sup>3</sup>, Dragana Božić<sup>3</sup>, Srđan Perišić<sup>1</sup>, Dušica Stojanović<sup>2</sup>, Petar Uskoković<sup>2</sup> <sup>1</sup>University of Belgrade, Innovation Centre of the Faculty of Technology and Metallurgy,

Belgrade, Belgrade, Serbia, <sup>2</sup>University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia, <sup>3</sup>University of Belgrade, Faculty of Pharmacy, Belgrade, Serbia

### P.S.II.E.6 3D Printable Polyhydroxyalkanoate Hydrogels as Potential Scaffolds for Cartilage Replacement

<u>Zuzana Kadlecová</u><sup>1</sup>, Nicole Černeková<sup>2</sup>, Adriána Kovalčík<sup>2</sup>, Lucy Vojtová<sup>1</sup> <sup>1</sup>Central European Research Institute, Brno University of Technology, Czechia, <sup>2</sup>Faculty of Chemistry, Brno University of Technology, Czechia

#### P.S.II.E.7 Feed additives based on polyvalent nanodisperse iron oxides, obtained by the electroerosion dispersion method, for feeding broiler chickens Tetiana Prikhna<sup>1</sup>, Mykola Monastyrov<sup>1</sup>, Olena Prysiazhna<sup>1</sup>, <u>Iryna Galstian<sup>2</sup></u>, Fernand Marquis<sup>3</sup>, Vasyl Kovalenko<sup>4</sup>, Mykola Novohatskyi<sup>5</sup>, Branko Matović<sup>6</sup>, Ivana Cvijović-Alagić<sup>6</sup>, Jerzy Madej<sup>7</sup>

<sup>1</sup>V. Bakul Institute for Superhard Materials of the National Academy of Sciences of Ukraine, Kiev, Ukraine, <sup>2</sup>G. V. Kurdyumov Institute for Metal Physics of the N.A.S. of Ukraine, Kyiv, Ukraine, <sup>3</sup>San Diego State University, San Diego, United States, <sup>4</sup>National University of Life and Environmental Science of Ukraine, <sup>5</sup>Leonid Pogorilyy Ukrainian Scientific Research Institute of Forecasting and Testing of Machinery and Technologies for Agricultural Production of the Ministry of Economy of Ukraine, Doslidnytske, Ukraine, <sup>6</sup>MSL, Vinča Institute of Nuclear Sciences, University of Belgrade, Serbia, <sup>7</sup>LLC "New Heating Technology", Bytom, Poland

### **P.S.II.E.8** SrTiO<sub>3</sub>-based nanoparticles in dental poly(methyl methacrylate): mechanical and thermal properties

Houda Taher Elhmali<sup>1</sup>, <u>Ivana Stajcic<sup>2</sup></u>, Milos Petrovic<sup>1</sup>, Aleksandar Stajcic<sup>3</sup>, Marija Jovanovic<sup>1</sup>, Dusica B. Stojanovic<sup>1</sup>, Petar Uskokovic<sup>1</sup>, Vesna Radojevic<sup>1</sup> <sup>1</sup>Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia, <sup>2</sup>Department of Physical Chemistry, "Vinča" Institute of Nuclear Sciences-National Institute of the Republic of Serbia, University of Belgrade, Serbia, <sup>3</sup>Center for Microelectronic Technologies, Institute of Chemistry, Technology and Metallurgy-National Institute of the Republic of Serbia, University of Belgrade, Serbia

### **P.S.II.E.9** Electroconductive electrospun PCL-MXene scaffolds for effective cardiac tissue regeneration

<u>Oleksiy Gogotsi</u><sup>1</sup>, Kateryna Diedkova<sup>2,3</sup>, Yevheniia Husak<sup>2,4</sup>, Wojciech Simka<sup>4</sup>, Viktoriia Korniienko<sup>2,3</sup>, Bojan Petrovic<sup>5</sup>, Anton Roshchupkin<sup>2</sup>, Agnieszka Stolarczyk<sup>4</sup>, Natalia Waloszczyk<sup>5</sup>, Ilya Yanko<sup>2</sup>, Kaspars Jekabsons<sup>3</sup>, Maria Čaplovičová<sup>6</sup>, Alexander D. Pogrebnjak<sup>2,6</sup>, Veronika Zahorodna<sup>1</sup>, Serhii Dukhnovskiy<sup>1</sup>, Iryna Roslyk<sup>1</sup>, Ivan Baginskiy<sup>1,2</sup>, Marko Radovic<sup>5</sup>, Sanja Kojic<sup>5</sup>, Una Riekstina<sup>3</sup>, Maksym Pogorielov<sup>2,3</sup> <sup>1</sup>Materials Research Centre, Kyiv, Ukraine; <sup>2</sup>Sumy State University, Sumy, Ukraine; <sup>3</sup>University of Latvia, Riga, Latvia; <sup>4</sup>Silesian University of Technology, Gliwice, Poland; <sup>5</sup>University of Novi Sad, Serbia; <sup>6</sup>Slovak University of Technology in Bratislava, Slovakia

### P.S.II.E.10 Multi-ion-doped mesoporous bioactive glass particles as fillers in 3D printed biocomposite scaffolds

<u>Tamara Matić</u><sup>1</sup>, Teodora Jakovljević<sup>1</sup>, Vukašin Ugrinović<sup>2</sup>, Miloš Papić<sup>3</sup>, Đorđe Janaćković<sup>1</sup>, Rada Petrović<sup>1</sup>, Biljana Ljujić<sup>3</sup>, Đorđe Veljović<sup>1</sup> <sup>1</sup>University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia, <sup>2</sup>Innovation Center of the Faculty of Technology and Metallurgy Ltd, Belgrade Serbia, <sup>3</sup>University of Kragujevac, Faculty of Medical Sciences, Kragujevac, Serbia

#### WRTCS

#### P.S.II.W.5 Processing of boron carbide ceramic reinforced with silicon carbide whiskers Branko Matović, Aleksa Luković

Centre of Excellence-CextremeLab, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia

### **P.S.II.W.6** Structure and dielectric behavior of BNT-BT piezoceramics obtained by hydrothermally synthesized powders

Andrea Lazić<sup>1</sup>, Jelena Vukmirović<sup>1</sup>, <u>Iva Toković<sup>1</sup></u>, Marija Milanović<sup>1</sup>, Branimir Bajac<sup>2</sup>, Elvira Toth<sup>3</sup>, Zeljka Cvejić<sup>3</sup>, Vladimir V. Srdić<sup>1</sup>

<sup>1</sup>Faculty of Technology Novi Sad, University of Novi Sad, Novi Sad, Serbia, <sup>2</sup>Institute Biosense, University of Novi Sad, Novi Sad, Serbia, <sup>3</sup>Faculty of Sciences, University of Novi Sad, Novi Sad, Serbia

### **P.S.II.W.7** The impact of sintering parameters on the physical properties of ceramic samples obtained by andesite basalt powder

<u>Vladimir Pavkov</u><sup>1</sup>, Gordana Bakić<sup>2</sup>, Vesna Maksimović<sup>1</sup>, Aleksandar Maslarević<sup>2</sup>, Bratislav Rajičić<sup>2</sup>, Nenad Milošević<sup>2</sup>, Aleksa Luković<sup>1</sup> <sup>1</sup>Department of Materials Science, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia, <sup>2</sup>Faculty of Mechanical Engineering, University of Belgrade, Belgrade, Serbia

### P.S.II.W.8 High-temperature humidity sensing ability of rare-earth-doped barium cerate

<u>Aleksandar Malešević</u>, Aleksandar Radojković, Jelena Mitrović, Milan Žunić, Olivera Zemljak, Sanja Perać, Zorica Branković, Goran Branković University of Belgrade, Institute for Multidisciplinary Research, Center of Excellence for Green Technologies, Belgrade, Serbia

#### P.S.II.W.9 Sintering behavior of Mo-based metal-matrix composite <u>levgen Solodkyi<sup>1,2</sup></u>, Manja Krüger<sup>1</sup>

<sup>1</sup>Otto von Guericke University Magdeburg, Magdeburg Germany, <sup>2</sup>Igor Sikorsky Kyiv Polytechnic Institute, Kyiv, Ukraine

Second YUCOMAT Plenary Session, Main Conference Hall

Session: 10<sup>00</sup> - 13<sup>00</sup>

### **Chairpersons: Sotiris E. Pratsinis, Patrice Simon and Ehrenfried Zschech** 10<sup>00</sup> - 10<sup>40</sup> Y.PL.S.II.4

### From aerosol synthesis of materials and devices to a new value for the mean free path of air

<u>Sotiris E. Pratsinis</u> Particle Technology Laboratory ETH Zürich, Zürich, Switzerland

#### 10<sup>40</sup> - 11<sup>20</sup> Y.PL.S.II.5

#### Probing the ion flux at the nanoscale with operando technologies

Kangkang Ge<sup>1</sup>, Jeronimo Miranda-Castro<sup>1</sup>, Audrey Perju<sup>1</sup>, B. Mondal<sup>1</sup>, Pierre-Louis Taberna<sup>1</sup>, Patrice Simon<sup>1,2</sup>

<sup>1</sup>Université Paul Sabatier, CIRIMAT UMR CNRS 5085, Toulouse, France; <sup>2</sup>Réseau sur le Stockage Electrochimique de l'Energie (RS2E), FR CNRS 3459, France

#### 11<sup>20</sup> - 12<sup>00</sup> Y.PL.S.II.6

### X-ray microscopy at electrochemical systems for sustainable energy technologies

Ehrenfried Zschech

Brandenburg University of Technology Cottbus-Senftenberg, Cottbus, Germany

#### 12<sup>00</sup> - 12<sup>40</sup> Y.PL.S.II.7

#### **Creation and Characterization of Nanopores in Hexagonal Boron Nitride via Aberration-Corrected Scanning Transmission Electron Microscopy** Rachael Keneipp<sup>1</sup>, Pia Bhatia<sup>1</sup>, Jordan Gusdorff<sup>2,3</sup>, Lee Bassett<sup>3</sup>, Marija Drndić<sup>1</sup>

<sup>1</sup>Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA, USA, <sup>2</sup>Department of Material Science and Engineering, University of Pennsylvania, Philadelphia, PA, USA, <sup>3</sup>Department of Electrical and Systems Engineering, University of Pennsylvania, Philadelphia, PA, USA

#### 12<sup>40</sup> - 13<sup>00</sup> Sponsor lecture:

#### U.S. Air force office of scientific research grant funding opportunities David Swanson

U.S. Air Force Office of Scientific Research, European Office of Aerospace Research and Development

13<sup>00</sup> - 15<sup>00</sup> Break

#### First WRTCS Oral Session, Main Conference Hall

#### Competition for the best oral presentation of young researchers

Session: 15<sup>00</sup> - 16<sup>30</sup>

#### Chairpersons: Biljana Stojanović, Đorđe Janaćković

15<sup>00</sup> - 15<sup>15</sup> **O.S.I.W.1** 

#### **Fabrication of High Entropy Alloys and Carbides via spark plasma sintering** <u>Daniel Valášek<sup>1</sup></u>, David Salamon<sup>1,2</sup>

<sup>1</sup>Department of Advanced Ceramic Materials, CEITEC Brno University of Technology, Purkyňova 123, Brno, Czech Republic, <sup>2</sup>Department of Materials Science, Montanuniversitat Leoben, Leoben, Austria

#### 15<sup>15</sup> - 15<sup>30</sup> **O.S.I.W.2**

### Bulk Ti and Ti<sub>6</sub>Al<sub>4</sub>V through Consolidation of Chips by Severe Plastic Deformation Methods

<u>Peter Cengeri<sup>2</sup></u>, Jelena Horky<sup>1</sup>, Laszlo Sajti<sup>1</sup>, Michael J. Zehetbauer<sup>2</sup>, Bartosz Sulkowski<sup>3</sup>, Grzegorz Boczkal<sup>3</sup>, Erhard Schafler<sup>2</sup>

<sup>1</sup>RHP-Technology GmbH, Seibersdorf, Austria, <sup>2</sup>Faculty of Physics, University of Vienna, Wien, Austria, <sup>3</sup>Department of Materials Science & Non-Ferrous Metals Engineering, Faculty of Non-Ferrous Metals, AGH University of Cracov, Krakow, Poland

#### 15<sup>30</sup> - 15<sup>45</sup> **O.S.I.W.3**

### Thermal stress analysis on thinning and new structure of Cu Clips attached with Ag sintered layers for high performance SiC chip systems

<u>Daito Murakami</u><sup>1</sup>, Masaaki Aoki<sup>1,2</sup>, Kazuma Yamashita<sup>1</sup>, Maurizio Fenech<sup>3</sup>, Riski Wirawan<sup>3</sup>, Nobuhiko Nakano<sup>1</sup>

<sup>1</sup>Department of Electronics and Electrical Engineering, Faculty of Science and Technology, Keio University, Yokohama, Kanagawa, Japan, <sup>2</sup>MacDermid Alpha Electronics Solutions/MacDermid Performance Solutions Japan, <sup>3</sup>Semiconductor Assembly Solutions/MacDermid Alpha Electronics Solutions

#### 15<sup>45</sup> - 16<sup>00</sup> **O.S.I.W.4**

#### Ti<sub>3</sub>C<sub>2</sub>Tx MXene surface exploitation for the practical applications

<u>Simonas Ramanavicius</u><sup>1</sup>, A. Popov<sup>2</sup>, S. Zukauskas<sup>3</sup>, S Adomaviciūtė-Grabusove<sup>4</sup>, M. Talaikis<sup>1</sup>, V. Sablinskas<sup>4</sup>, O. Gogotsi<sup>5</sup>, Y. Gogotsi<sup>6</sup>, G. Niaura<sup>1</sup>, A. Ramanaviciene<sup>2</sup>, A. Ramanavicius<sup>3</sup>

<sup>1</sup>State Research Institute Center for Physical Sciences and Technology (FTMC), Vilnius, Lithuania, <sup>2</sup>NanoTechnas-Center of Nanotechnology and Materials Science, Faculty of Chemistry and Geosciences, Vilnius University, Vilnius, Lithuania, <sup>3</sup>Department of Physical Chemistry, Faculty of Chemistry and Geosciences, Institute of Chemistry, Vilnius University, Lithuania, <sup>4</sup>Institute of Chemical Physics, Vilnius University, Vilnius, <sup>5</sup>Materials Research Center Ltd., Ukraine, <sup>6</sup>Department of Materials Science and Engineering and A.J. Drexel Nanomaterials Institute, Drexel University, Philadelphia, PA, USA

#### 16<sup>00</sup> - 16<sup>15</sup> O.S.I.W.5

**Investigation of a UO**<sub>2</sub> ceramic as a reference for a homogeneous MOX fuel Kaythleen Torrente<sup>1</sup>, C. Duguay<sup>2</sup>, F. Doreau<sup>1</sup>, G. Bernard-Granger<sup>1</sup> <sup>1</sup>CEA, DES, ISEC, DMRC, Univ. Montpellier, Marcoule, France, <sup>2</sup>CEA, DES, IRESNE, DEC, Cadarache, France

#### 16<sup>15</sup>- 16<sup>30</sup> **O.S.I.W.6**

#### **Preparation of single-phase high entropy ceramic for further modification: Comparison of different sintering processes**

<u>Marek Rotter</u><sup>1</sup>, Katarína Drdlíková<sup>2</sup>, Karel Maca<sup>1,2</sup> <sup>1</sup>CEITEC, Brno University of Technology, Brno, Czech Republic, <sup>2</sup>Faculty of Mechanical Engineering, Brno University of Technology, Technicka 2, Brno, Czech Republic

#### Second WRTCS Oral Session, Main Conference Hall

Session: 16<sup>30</sup> - 17<sup>30</sup>

#### Chairpersons: Elena Pereloma, Masaaki Aoki

16<sup>30</sup> - 16<sup>45</sup> **O.S.II.W.7** 

### Thermal stress and deformation in SiC semiconductor chip systems having three-layer stacked Clips attached by Ag sintered layers

<u>Masaaki Aoki<sup>1,2</sup>,</u> Kazuma Yamashita<sup>1</sup>, Maurizio Fenech<sup>3</sup>, Riski Wirawan<sup>3</sup>, Nobuhiko Nakano<sup>1</sup>

<sup>1</sup>Department of Electronics and Electrical Engineering, Faculty of Science and Technology, Keio University, Yokohama, Kanagawa, Japan, <sup>2</sup>MacDermid Alpha Electronics Solutions / MacDermid Performance Solutions Japan, <sup>3</sup>Semiconductor Assembly Solutions / MacDermid Alpha Electronics Solutions

#### 16<sup>45</sup> - 17<sup>00</sup> **O.S.II.W.8**

Success and failure of in-situ microstructure observations in metastable  $\boldsymbol{\beta}$  Ti alloys

Frank Niessen<sup>1,2</sup>, Ryan Naseri<sup>1</sup>, Azdiar A. Gazder<sup>1</sup>, Dmytro Savvakin<sup>3</sup>, <u>Elena</u> <u>Pereloma<sup>1,4</sup></u>

<sup>1</sup>UOW Electron Microscopy Centre, University of Wollongong, Wollongong, NSW, Australia, <sup>2</sup>Section of Materials and Surface Engineering, Department of Civil and Mechanical Engineering, Technical University of Denmark, Kongens Lyngby, Denmark, <sup>3</sup>Institute for Metal Physics, National Academy of Sciences of Ukraine, Kyiv, Ukraine, <sup>4</sup>School of Mechanical, Materials, Mechatronic and Biomedical Engineering, University of Wollongong, NSW, Australia

#### 17<sup>00</sup>- 17<sup>15</sup> **O.S.II.W.9**

#### Reactive sintering behavior and enhanced densification of diboridecarbide composites

<u>Sijia Huo</u>, Yujin Wang, Lei Chen, Yu Zhou

School of Material Science and Engineering, Harbin Institute of Technology, China 17<sup>15</sup>- 17<sup>30</sup> O.S.II.W.10

#### Entropy as an Order Parameter in Thermodynamics

Yuri Kornyushin, Maître Jean Brunschvig Research Unit, Jerusalem, Israel

#### Thursday, September 5, 2024

Third YUCOMAT Poster Session, National Restaurant Jadranka Terrace Session: 08<sup>00</sup> - 09<sup>45</sup> Chairpersons: Sonja Jovanović, Ivana Dinić

#### YUCOMAT SYMPOSIUM A:

ADVANCED METHODS IN SYNTHESIS AND PROCESSING OF MATERIALS

P.S.III.A.8 Sustainable synthesis of Ni(II) complex with 3,5-pyrazoledicarboxylic acid as ligand via mechanochemistry

<u>Nina Jovović</u>, Željko Jaćimović, Milica Kosović Perutović University of Montenegro, Faculty of Metallurgy and Technology, Cetinjski put bb, 81000 Podgorica, Montenegro

#### P.S.III.A.9 Solidification curves of Al-Cu-Mg alloys

<u>Biljana Zlatičanin</u><sup>1</sup>, Branislav Radonjić <sup>1</sup>Faculty of Metallurgy and Technology, Cetiniski put bb. Podgorica, Montenegro

#### P.S.III.A.10 Double hot dip ZnAl coatings on reinforcement steel

<u>Anżelina Marek<sup>1</sup></u>, Veronika Steinerová<sup>2,3</sup>, Petr Pokorný<sup>2</sup>, Henryk Kania<sup>1</sup> <sup>1</sup>Silesian University of Technology, Faculty of Materials Engineering, Gliwice, Poland, <sup>2</sup>Czech Technical University, Faculty of Architecture, <sup>3</sup>Czech Technical University, Klokner Institute, Prague, Czech Republic

### P.S.III.A.11 Cost-efficient method for obtaining magnetic materials by processing iron-containing liquid waste

<u>Gennadii Kochetov</u>, Dmytro Samchenko, Oles Lastivka *Kyiv National University of Construction and Architecture, Ukraine* 

#### YUCOMAT SYMPOSIUM B:

#### ADVANCED MATERIALS FOR HIGH-TECHNOLOGY APPLICATION

#### P.S.III.B.12 Full cell sodium storage performance of biomass-derived nongraphitizable carbon

Jana Mišurović<sup>1</sup>, Aleksandra Gezović Miljanić<sup>1</sup>, Alen Vižintin<sup>2</sup>, Veselinka Grudić<sup>1</sup>, Robert Dominko<sup>2</sup>, Milica Vujković<sup>3,4</sup>

<sup>1</sup>University of Montenegro - Faculty of Metallurgy and Technology, Podgorica, Montenegro, <sup>2</sup>National Institute of Chemistry, Ljubljana, Slovenia, <sup>3</sup>University of Belgrade - Faculty of Physical Chemistry, Belgrade, Serbia, <sup>4</sup>Center for Interdisciplinary and Multidisciplinary Studies, University of Montenegro, Podgorica, Montenegro

### P.S.III.B.13 Influence of build orientation and different printing angles on impact toughness of carbon-reinforced PET-G FDM material

<u>Milovan Paunić</u><sup>1</sup>, Aleksandar Sedmak<sup>1</sup>, Milan Janković<sup>1</sup>, Sergiu-Valentin Galațanu<sup>2</sup>, Horia Dascau<sup>3</sup>, Igor Balać<sup>1</sup>

<sup>1</sup>University of Belgrade, Faculty of Mechanical Engineering, Belgrade, Serbia, <sup>2</sup>Polytechnic University of Timişoara, Department of Mechanics and Strength of Materials, Mihai Viteazu Avenue, Timişoara, Romania, <sup>3</sup>ISIM, Mihai Viteazu Avenue, Timişoara, Romania

### P.S.III.B.14 High-performance hydrophilic separators for supercapacitors based on alkali-modified cellulose nanocrystal aerogels

Daniel Mijailović<sup>1</sup>, Patrick Gane<sup>1,2</sup>, Katarina Dimić-Mišić<sup>2</sup>, Monireh Imani<sup>2</sup>, Dušica Stojanović<sup>1</sup>, Vesna Radojević<sup>1</sup>, Petar Uskoković<sup>1</sup> <sup>1</sup>University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia, <sup>2</sup>Department of Bioproducts and Biosystems, School of Chemical Engineering, Aalto University, Aalto, Finland

#### P.S.III.B.15 Crystal structure, X-ray spectroscopic properties and Mössbauer spectra of TaFeP <u>Ivan Shcherba<sup>1</sup></u>, Henrik Noga<sup>2</sup>, Victor Antonov<sup>3</sup>, Olga Zhak<sup>1</sup>,

Kamila Komedera<sup>2</sup>, Dragan Uskoković<sup>4</sup>, Lev Bekenov<sup>3</sup>, Bohdan Jatsyk<sup>5</sup>, Kateryna Starushenko<sup>1</sup>, Yulija Nykyruy<sup>1</sup>

<sup>1</sup>Ivan Franko National University of Lviv, Lviv, Ukraine, <sup>2</sup>Institute of Technology, University of the NEC, Krakow, Poland, <sup>3</sup>G. V. Kurdyumov Institute for Metal Physics of the N.A.S.A., Ukraine, <sup>4</sup>Institute of Technical Sciences of SASA, Belgrade, Serbia, <sup>5</sup>Lviv National University of Veterinary Medicine and Biotechnologies, Ukraine

### P.S.III.B.16 Determination of optimal conditions of non-linear optical interactions in monoclinic crystals

<u>Anatoliy Andrushchak</u><sup>1</sup>, Dmytro Shulga<sup>1</sup>, Oleg Buryy<sup>1</sup>, Bouchta Sahraoui<sup>2</sup> <sup>1</sup>Lviv Polytechnic National University, Lviv, Ukraine, <sup>2</sup>University of Angers, LPhiA, SFRMATRIX, Angers, France

#### YUCOMAT SYMPOSIUM C: NANOSTRUCTURED MATERIALS

P.S.III.C.14 Carbonization of MOF-5/Polyaniline and ZIF-67/Polyaniline to Zn/N,Odoped and Co/N,O-doped carbon composites with high specific capacitance Marjetka Savić<sup>1</sup>, Aleksandra Janošević Ležaić<sup>2</sup>, Maja Ranković<sup>3</sup>,

Nemanja Gavrilov<sup>3</sup>, Igor Pašti<sup>3</sup>, Gordana Ćirić-Marjanović<sup>3</sup>

<sup>1</sup>Vinča Institute of Nuclear Science, University of Belgrade, National Institute of the Republic of Serbia, Belgrade, Serbia, <sup>2</sup>University of Belgrade-Faculty of Pharmacy, Belgrade, Serbia, <sup>3</sup>University of Belgrade-Faculty of Physical Chemistry, Belgrade, Serbia

### P.S.III.C.15 Oxidation resistance and electrical conductivity of nanostructured coatings for titanium interconnects of solid oxide fuel cell

<u>Viktoriya Podhurska</u><sup>1</sup>, Orest Ostash<sup>1</sup>, Mykola Kuzmenko<sup>2</sup>, Oleksander Kuprin<sup>3</sup> <sup>1</sup>Karpenko Physico-Mechanical Institute of the NAS of Ukraine, Lviv, Ukraine, <sup>2</sup>Institute for Problems of Materials Science of the NAS of Ukraine, Kyiv, Ukraine, <sup>3</sup>National Science Center "Kharkiv Institute of Physics and Technology" of the NAS of Ukraine, Kharkiv, Ukraine

### P.S.III.C.16 Waterborne polyurethane nanocomposite reinforced by chitin glucan nanocrystals

<u>Beata Strachota</u>, Silvia Mares Barbosa, Adam Strachota, Ewa Pavlova, Magdalena Konefał, Jiří Hodan

Institute of Macromolecular Chemistry, Czech Academy of Sciences, Praha 6, Czech Republic

### P.S.III.C.17 Facile synthesis of CoAu/rGO nanocomposite for sensing of As<sup>3+</sup> ions in neutral medium

<u>Kristina Radinović</u><sup>1</sup>, Jadranka Milikić<sup>1</sup>, Nemanja Gavrilov<sup>1</sup>, Dalibor Stanković<sup>2</sup>, Aleyna Basak<sup>3</sup>, Önder Metin<sup>3,4</sup>, Biljana Šljukić<sup>1,5</sup>

<sup>1</sup>University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia, <sup>2</sup>University of Belgrade, Faculty of Chemistry, Belgrade, Serbia, <sup>3</sup>Department of Chemistry, College of Sciences, Koç University, Istanbul, Türkiye, <sup>4</sup>Koç University Surface Science and Technology Center (KUYTAM), Sarıyer, Istanbul, Türkiye, <sup>5</sup>Center of Physics and Engineering of Advanced Materials, Laboratory for Physics of Materials and Emerging Technologies, Chemical Engineering Department, Instituto Superior Técnico, Universidade de Lisboa, Lisbon, Portugal

#### P.S.III.C.18 Ti<sub>3</sub>C<sub>2</sub>Tx MXenes: enhancing performance in glucose biosensors

<u>Anton Popov<sup>1,2</sup></u>, Viktorija Lisyte<sup>2</sup>, Marina Sapauskiene<sup>2</sup>, Asta Kausaite-Minkstimiene<sup>1,2</sup>, Almira Ramanaviciene<sup>1,2</sup>

<sup>1</sup>Department of Immunology and Bioelectrochemistry, State Research Institute Centre for Innovative Medicine, Vilnius, Lithuania, <sup>2</sup>NanoTechnas - Center of Nanotechnology and Materials Science, Faculty of Chemistry and Geosciences, Vilnius University, Lithuania

### P.S.III.C.19 Niobium MXenes with lanthanum: electrochemical performance in microsupercapacitors

<u>Meriene Gandara</u><sup>1</sup>, Bianca Fortes Palley<sup>1</sup>, Lazar Rakočević<sup>2</sup>, Dušan Mladenović<sup>3</sup>, Biljana Šljukić<sup>3,4</sup>, Emerson Sarmento Gonçalves<sup>1,5</sup> <sup>1</sup>Technological Institute of Aviation, Space Science and Technology Graduate Program, São José dos Campos, Brazil, <sup>2</sup>Vinča Institute of Nuclear Sciences, Department of Atomic Physics, Belgrade, Serbia, <sup>3</sup>University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia, <sup>4</sup>Center of Physics and Engineering of Advanced Materials, Laboratory for Physics of Materials and Emerging Technologies, Chemical Engineering Department, Instituto Superior Técnico, Universidade de Lisboa, Portugal, <sup>5</sup>Institute of Aeronautics and Space, Divisão de Materiais, Praça Marechal Eduardo Gomes, São José dos Campos, Brazil

### P.S.III.C.20 Microstructural transformation of SPD processed Al-Li alloys during low temperatures deformation

<u>Sergii Shumilin</u><sup>1</sup>, Tetiana Hryhorova<sup>1</sup>, Pavel Zabrodin<sup>1,2</sup>, Daria Drozdenko<sup>3</sup> <sup>1</sup>B. Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine, Kharkiv, Ukraine, <sup>2</sup>Czech Academy of Sciences, Institute of Theoretical and Applied Mechanics, Prague, Czech Republic, <sup>3</sup>Charles University, Faculty of Mathematics and Physics, Department of Physics of Materials, Prague, Czech Republic

### P.S.III.C.21 Nanoscale assessment of free volume in BaGa<sub>2</sub>O<sub>4</sub> ceramics doped with Eu<sup>3+</sup> ions using PAL spectroscopy

Halyna Klym<sup>1</sup>, Yuriy Kostiv<sup>1</sup>, Oleksii Kushnir<sup>2</sup>

<sup>1</sup>Lviv Polytechnic National University, Lviv, Ukraine, <sup>2</sup>Ivan Franko National University of Lviv, Lviv, Ukraine

#### YUCOMAT SYMPOSIUM D: ECO-MATERIALS AND ECO-TECHNOLOGIES

P.S.III.D.7 Modification of ZnO surfaces with oxygen vacancies: density functional study Jelena Belošević-Čavor, Vasil Koteski, Valentin Ivanovski, Ana Umićević, Dragan Toprek, Ana Kapidžić

Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia

### P.S.III.D.8 Swelling behaviour and heavy metals adsorption on alginate-based hydrogels filled with LaponiteRD and montmorillonite

<u>Olena Goncharuk<sup>1,2</sup></u>, Nataliia Guzenko<sup>1</sup>, Yurii Samchenko<sup>2</sup>, Svitlana Dybkova<sup>2</sup>, Katarzyna Szewczuk-Karpisz<sup>1</sup>

<sup>1</sup>Institute of Agrophysics, Polish Academy of Sciences, Lublin, Poland, <sup>2</sup>Ovcharenko Institute of Biocolloidal Chemistry of NAS of Ukraine, Kyiv, Ukraine

P.S.III.D.9 Sky Harvesting with Sustainable Materials: NOx Mitigation through Air Mining applying Ambient Air Pollution Simulation and Kinetic Modelling <u>Nemanja Barać<sup>1</sup></u>, Katarina Dimić-Mišić<sup>2</sup>, Mirko Stijepović<sup>3</sup>, Mirjana Kijevčanin<sup>3</sup>, Monireh Imani<sup>2</sup>, Petar Uskoković<sup>3</sup>, Djordje Janaćković<sup>3</sup>, Ernesto Barceló<sup>2,4</sup>, Patrick Gane<sup>2,3</sup>

> <sup>1</sup>Innovation Center of Faculty of Technology and Metallurgy in Belgrade Ltd., Belgrade, Serbia, <sup>2</sup>School of Chemical Engineering, Department of Bioproducts and Biosystems, Aalto University, Aalto, Helsinki, Finland, <sup>3</sup>Faculty of Technology and Metallurgy, University of Belgrade, , Belgrade, Serbia, <sup>4</sup>Environmental, Social and Governance, Gestamp Automoción S.A., Madrid, Spain

#### YUCOMAT SYMPOSIUM E: BIOMATERIALS

#### P.S.III.E.11 Novel Hybrid Poly(methacrylic acid)/Gelatin/Alginate Hydrogels for Bone and Cartilage Tissue Engineering

<u>Vukasin Ugrinović</u><sup>1</sup>, Maja Marković<sup>1</sup>, Vesna Panić<sup>1</sup>, Đorđe Veljović<sup>2</sup> <sup>1</sup>Innovation Center of Faculty of Technology and Metallurgy, Belgrade, Serbia, <sup>2</sup>Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia

### P.S.III.E.12 Acrylate functional composites reinforced using the ZnAl layered double hydroxide

Marija Jovanović<sup>1</sup>, Vladislav Tadić<sup>1</sup>, Marija Vuksanović<sup>2</sup>, Miloš Petrović<sup>1</sup>, Vesna Radojević<sup>1</sup>, <u>Radmila Jančić Heinemann<sup>1</sup></u>

<sup>1</sup>Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia, <sup>2</sup>Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia

#### P.S.III.E.13 Ti<sub>3</sub>C<sub>2</sub> MXene-Based Electroconductive Polymer Nerve Guidance Conduits for Regeneration of Peripheral Nerve Injuries

Inna Chorna<sup>1</sup>, Sergiy Kyrylenko<sup>1</sup>, Kateryna Diedkova<sup>2</sup>, Zhanna Klishchova<sup>1,3</sup>, Serhii Dukhnovskiy<sup>4</sup>, Ivan Baginskiy<sup>4</sup>, Veronika Zahorodna<sup>4</sup>, Iryna Roslyk<sup>4</sup>, Oleksiy Gogotsi<sup>4</sup>, Paola Caro<sup>5</sup>, Alexandre Oliveira<sup>5</sup>, Maksym Pogorielov<sup>1,2</sup> <sup>1</sup>Biomedical Research Center, Sumy State University, Sumy, Ukraine, <sup>2</sup>Institute of Atomic Physics and Spectroscopy, University of Latvia, Riga, Latvia, <sup>3</sup>Federal University of Lavras UFLA, Lavras, MG, Brazil, <sup>4</sup>Carbon Ukraine Ltd, Kyiv, Ukraine; <sup>5</sup>University of Campinas UNICAMP, Campinas, SP, Brazil

## **P.S.III.E.14** In-line X-ray phase-contrast imaging of a bamboo splinter

<u>Pavel Zabrodin 1,2,</u> Daniel Vavřík<sup>1</sup>, Pavel Beneš<sup>1</sup>, Jan Žemlička<sup>3</sup> <sup>1</sup>The Czech Academy of Sciences, Institute of Theoretical and Applied Mechanics, Praha, Czech Republic, <sup>2</sup>B. Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine, Kharkiv, Ukraine, <sup>3</sup>Institute of Experimental and Applied Physics, Czech Technical University in Prague, Praha, Czech Republic

# P.S.III.E.15 The corrosion resistance of the nanostructured modified ultrafine-grained titanium in Ringer's solution

Dragana Mihajlović<sup>1</sup>, Jelena Bajat<sup>1</sup>, Veljko Đokić<sup>1,2</sup>

<sup>1</sup>University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia, <sup>2</sup>Innovation Centre of Faculty of Technology and Metallurgy, Belgrade, Serbia

### P.S.III.E.16 Si-modified biogenic hydroxyapatite/alginate hydrogel composites: structure and properties

Yuri Samchenko<sup>1</sup>, <u>Olena Sych<sup>2,3</sup></u>, Nataliia Pinchuk<sup>2,4</sup>, Liudmyla Kernosenko<sup>1</sup>, Svitlana Stelmakh<sup>3</sup>, Jan Mizeracki<sup>3</sup>, Pavlo Vorotytskyi<sup>1</sup>, Tetiana Poltoratska<sup>1</sup>, Anna Synytsia<sup>2</sup>, Ganna Chyzhyk<sup>5,7</sup>, Yuliia Vronska<sup>6,7</sup>

<sup>1</sup>F.D. Ovcharenko Institute of Biocolloidal Chemistry of NAS of Ukraine, Kyiv, Ukraine, <sup>2</sup>Frantsevich Institute for Problems of Materials Science of NAS of Ukraine, Kyiv, Ukraine, <sup>3</sup>Institute of High Pressure Physics of the PAS, Warsaw, Poland, <sup>4</sup>Institute of Low Temperature and Structure Research of the PAS, Wrocław, Poland, <sup>5</sup>G.S. Pisarenko Institute for Problems of Strength of NAS of Ukraine, Kyiv, Ukraine, <sup>6</sup>G.V. Kurdyumov Institute for Metal Physics NAS of Ukraine, Kyiv, Ukraine, <sup>7</sup>Institute of Metallurgy and Materials Science of the PAS, Krakow, Poland

# P.S.III.E.17 The use of very fast solid-state NMR spectroscopy and DFT calculations to design the microstructure of alginate chains cross-linked by paramagnetic ions

<u>Martina Urbanova<sup>1</sup></u>, Libor Kobera<sup>1</sup>, Miroslava Pavelkova<sup>2</sup>, Katerina Kubova<sup>2</sup>, Jiri Brus<sup>1</sup>

<sup>1</sup>Department of NMR spectroscopy, Institute of Macromolecular Chemistry, Czech Academy of Sciences, Czech Republic, <sup>2</sup>Department of Pharmaceutical Technology, Faculty of Pharmacy, Masaryk University Brno, Czech Republic

# P.S.III.E.18 Structure and dynamics of multicomponent polycrystalline materials at atomic resolution

Jiri Brus, Martina Urbanova, Jiri Czernek, Jakub Obuch Department of NMR spectroscopy, Institute of Macromolecular Chemistry, Czech Academy of Sciences, Czech Republic

### P.S.III.E.19 Improved solubility and certain ratio of tautomeric forms of curcumin in the nanoformulations with alkylammonium dimeric surfactants Olga Kazakova, Natalia Lipkovska, Valentyna Barvinchenko

Chuiko Institute of Surface Chemistry, NAS of Ukraine, Kyiv, Ukraine

# P.S.III.E.20 Combined antimicrobial effect of nanoparticles and medicinal plants against multi-drug resistant microbes

<u>Viktoriia Holubnycha</u>, Anna Yanovska, Roman Pshenychnyi Sumy State University, Sumy, Ukraine

#### 25<sup>th</sup> YUCOMAT 2024 & XIII WRTCS Herceg Novi, September 2 - 6, 2024

Third YUCOMAT Plenary Session, Main Conference Hall Session: 10<sup>00</sup> - 12<sup>40</sup>

**Chairpersons: Hui-Ming Cheng, Xinliang Feng, Mark C. Hersam and Andrew M. Minor** 10<sup>00</sup> - 10<sup>40</sup> **Y.PL.S.III.8** 

### **Exploration of New 2D Materials and Their New Properties** <u>Hui-Ming Cheng</u>

Institute of Technology for Carbon Neutrality, Shenzhen Institute of Advanced Technology, Chinese Academy of Sciences, Shenzhen, China; Faculty of Materials Science and Energy Engineering, Shenzhen University of Advanced Technology, Shenzhen, China; Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang, China

# 10<sup>40</sup> - 11<sup>20</sup> Y.PL.S.III.9

Beyond Layers: Unveiling the Potential of Organic 2D Crystals in Emerging Material Science

Xinliang Feng

Max Planck Institute of Microstructure Physics and Technische Universitaet Dresden Y.PL.S.III.10

# 11<sup>20</sup> - 12<sup>00</sup> Y.PL.S.III.10

### **Low-Dimensional Neuromorphic Electronic Materials and Applications** <u>Mark C. Hersam</u>

Department of Materials Science and Engineering, Northwestern University, Evanston, IL, USA

# 12<sup>00</sup> - 12<sup>40</sup> Y.PL.S.III.11

### Imaging of short range order with electron microscopy: from high performance alloys to semiconductor thin films Andrew M. Minor

Department of Materials Science and Engineering, University of California, Berkeley, CA, 94720 USA. and the National Center for Electron Microscopy, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA, USA

14<sup>00</sup> - 19<sup>00</sup> Boat-trip around Boka Kotorska Bay

# Friday, September 6, 2024

Second YUCOMAT Oral Session, Main Conference Hall Session: 09<sup>00</sup> - 11<sup>45</sup>

Chairpersons: Brigita Hočevar, Patrick Gane

# YUCOMAT SYMPOSIUM A:

ADVANCED METHODS IN SYNTHESIS AND PROCESSING OF MATERIALS 09<sup>00</sup> - 09<sup>15</sup> O.S.II.A.1

# Oxygen plasma-induced dry production of micro nanofibrillated cellulose (MNFC)

<u>Patrick Gane<sup>1,2</sup></u>, Katarina Dimić-Mišić<sup>1</sup>, Monireh Imani<sup>1</sup>, Bratislav Obradović<sup>3</sup>, Milorad Kuraica<sup>3</sup>, Huy Quang Lê<sup>1</sup>, Matea Korica<sup>4</sup>, Mirjana Kostić<sup>2</sup>

<sup>1</sup>Aalto University, Department of Bioproducts and Biosystems, School of Chemical Engineering, Aalto, Helsinki, Finland, <sup>2</sup>University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia, <sup>3</sup>Faculty of Physics, University of Belgrade, Belgrade, Serbia, <sup>4</sup>Innovation Center of Faculty of Technology and Metallurgy Ltd., University of Belgrade, Belgrade, Serbia

## 09<sup>15</sup> - 09<sup>30</sup> **O.S.II.A.2**

Enhancing Selective Deoxydehydration of Biobased Compounds for Biobased Nylon Precursors Using Metal-Doped Solid Rhenium Catalysts Brigita Hočevar, Maja Gabrič, Rok Pogorevc, Žan Lavrič, Matej Huš, Miha Grilc, Blaž Likozar

Department of Catalysis and Chemical Reaction Engineering, National Institute of Chemistry, Ljubljana, Slovenia

## 09<sup>30</sup> - 09<sup>45</sup> O.S.II.A.3

### Integration of functional oxides with silicon substrate for photoelectrochemical water splitting

<u>Zoran Jovanović</u><sup>1,2</sup>, Urška Trstenjak<sup>2</sup>, Binbin Chen<sup>3</sup>, Darija Petković<sup>1</sup>, Gertjan Koster<sup>4</sup>, Matjaž Spreitzer<sup>2</sup>

<sup>1</sup>Laboratory of Physics, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia, <sup>2</sup>Advanced Materials Department, Jožéf Stefan Institute, Ljubljana, Slovenia, <sup>3</sup>Key Laboratory of Polar Materials and Devices (MOE) and Department of Electronics, East China Normal University, Shanghai, China, <sup>4</sup>MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands

## 0945 - 1000 O.S.II.A.4

## Synthesis and property of LaLuO<sub>3</sub>:Yb<sup>3+</sup> nanosize powders

Oksana Korniienko, Andrey Ragulya, Yuriy Yurchenko, Oleksandr Shyrokov, Tatiana Lobunets, Tamara Tomila, Marina Zamula, Valeriy Kolesnichenko Frantsevich Institute for Problem of Materials Science, NAS of Ukraine, Kyiv

### 10<sup>00</sup> - 10<sup>15</sup> **O.S.II.A.5**

# The influence of metal phase of novel $Al_2O_3/TiO_2/TiAl_2O_5$ composites obtained via slip casting method

<u>Marcin Wachowski</u><sup>1</sup>, Justyna Zygmuntowicz<sup>2</sup>, Robert Kosturek<sup>1</sup>, Lucjan Śnieżek<sup>1</sup>, Paulina Piotrkiewicz<sup>2</sup>, Radosław Żurowski<sup>3</sup>

<sup>1</sup>Faculty of Mechanical Engineering, Military University of Technology, Warsaw, Poland, <sup>2</sup>Faculty of Materials Science and Engineering, Warsaw University of Technology, Warsaw, Poland, <sup>3</sup>Faculty of Chemistry, Warsaw University of Technology, Warsaw, Poland

# YUCOMAT SYMPOSIUM B:

# ADVANCED MATERIALS FOR HIGH-TECHNOLOGY APPLICATION

# 10<sup>15</sup> - 10<sup>30</sup> **O.S.II.B.4**

# Alpha-pinene isomerization over TMAOH-treated multilayered Ti<sub>3</sub>C<sub>2</sub>Tx MXene

Bartosz Środa<sup>1</sup>, P. Miądlicki<sup>2</sup>, A. Wróblewska<sup>2</sup>, B. Zielińska<sup>1</sup>

<sup>1</sup>Department of Nanomaterials Physicochemistry, Faculty of Chemical Technology and Engineering, West Pomeranian University of Technology in Szczecin, Szczecin, Poland, <sup>2</sup>Department of Catalytic and Sorbent Materials Engineering, Faculty of Chemical Technology and Engineering, West Pomeranian University of Technology in Szczecin, Szczecin, Poland

### 10<sup>30</sup> - 10<sup>45</sup> **O.S.II.B.5**

# Insight into electrocatalytic oxygen evolution the reaction mechanism in the presence of Borophene/Ni<sup>2+</sup> with induced crystal lattice defects and porosity

<u>Ewa Mijowska</u>, Klaudia Zielinkiewicz, Grzegorz Leniec West Pomeranian University of Technology, Szczecin Faculty of Chemical Technology and Engineering, Department of Nanomaterials Physicochemistry, Szczecin, Poland

### 10<sup>45</sup> - 11<sup>00</sup> **O.S.II.B.6**

# Exploring the potential of $Na_4Fe_3(PO_4)_2P_2O_7/C$ as a cathode material for Na-ion rechargeable batteries

<u>Milica Vujković<sup>1,2</sup></u>, Aleksandra Gezović Miljanić<sup>3</sup>, Jana Mišurović<sup>3</sup>, Alen Vižintin<sup>4</sup>, Slavko Mentus<sup>1,5</sup>, Robert Dominko<sup>4</sup>

<sup>1</sup>University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia, <sup>2</sup>Center for Interdisciplinary and Multidisciplinary Studies, University of Montenegro, Podgorica, Montenegro, <sup>3</sup>Faculty of Metallurgy and Technology, University of Montenegro, Podgorica, Montenegro, <sup>4</sup>National Institute of Chemistry, Ljubljana, Slovenia, <sup>5</sup>Serbian Academy of Sciences and Arts, Belgrade, Serbia

### YUCOMAT SYMPOSIUM E: BIOMATERIALS

### 11<sup>00</sup> - 11<sup>15</sup> **O.S.II.E.5**

Laser-Induced Self-Organized Microrod Arrays for Osteoblasts Proliferation <u>Iaroslav Gnilitskyi<sup>1,2</sup></u>, K. Diedkova<sup>3,4</sup>, Anton Roshchupkin<sup>3</sup>, Milena Yalyzhko<sup>3</sup>, M. Pogorelov<sup>3,4</sup>, A. V. Zayats<sup>1</sup>

<sup>1</sup>Department of Physics and London Centre for Nanotechnology, King's College London, Strand, London, UK, <sup>2</sup>Department of Applied Physics, Lviv Polytechnic National University, Lviv, Ukraine, <sup>3</sup>Biomedical Research Center, Sumy State University, Sumy, Ukraine, <sup>4</sup>University of Latvia, Institute of Atomic Physics and Spectroscopy, Riga, Latvia

## 11<sup>15</sup> - 11<sup>30</sup> **O.S.II.E.6**

# Antibacterial effectiveness and safety of MXene-loaded electrospun polycaprolactone membranes for photothermal ablation

<u>Viktoriia Korniienko<sup>1,2</sup></u>, Keelan Warren<sup>1</sup>, Yuliia Varava<sup>2</sup>, Valeriia Korniienko<sup>2</sup>, Kateryna Diedkova<sup>1</sup>, Veronika Zahorodna<sup>3</sup>, Oleksiy Gogotsi<sup>3</sup>, Una Riekstina<sup>1</sup>, Maksym Pogorielov<sup>1,2</sup>

<sup>1</sup>University of Latvia, Riga, Latvia, <sup>2</sup>Sumy State University, Sumy, Ukraine, <sup>3</sup>CARBON-UKRAINE Ltd., Kiev, Ukraine

### 11<sup>30</sup> - 11<sup>45</sup> **O.S.II.E.7**

# *In vitro* electrophoresis to uncover mechanism of fragmentation of DNA by MXene in DNA comet assay

Inna Chorna<sup>1</sup>, Zhanna Klishchova<sup>1,2</sup>, Artem Shmatkov<sup>1</sup>, Anton Roshchupkin<sup>1</sup>, Illya Yanko<sup>1</sup>, Sergiy Dukhnovskiy<sup>3</sup>, Ivan Baginskiy<sup>3</sup>, Veronika Zahorodna<sup>3</sup>, Iryna Roslyk<sup>3</sup>, Oleksiy Gogotsi<sup>3</sup>, Maksym Pogorielov<sup>1,4</sup>, <u>Sergiy Kyrylenko<sup>1</sup></u> <sup>1</sup>Sumy State University, Sumy, Ukraine, <sup>2</sup>Federal University of Lavras UFLA, Lavras, Brazil, <sup>3</sup>Materials Research Centre LTD, Kyiv, Ukraine, <sup>4</sup>University of Latvia, Riga, Latvia

### 25<sup>th</sup> YUCOMAT 2024 & XIII WRTCS Herceg Novi, September 2 - 6, 2024

	)9ºº - 11ºº ons:     Carmen Lorena Manzanares-Palenzuela, Rastko Vasilić
	T SYMPOSIUM C: NANOSTRUCTURED MATERIALS
	O.S.III.C.4
	Advanced composite nanomaterials fabricated by high-pressure torsion technique
	<u>Piotr Bazarnik</u> <sup>1</sup> , Yi Huang <sup>2</sup> , Małgorzata Lewandowska <sup>1</sup> , Terence G. Langdon <sup>2</sup> <sup>1</sup> Warsaw University of Technology, Faculty of Materials Science, Poland, <sup>2</sup> Materials Research Group, Department of Mechanical Engineering, University of Southampton, UK
09 <sup>15</sup> - 09 <sup>30</sup>	Aqueous dispersions of basic Cu salts. Electric double layer and ion exchange
	<u>Marek Kosmulski</u> Lublin University of Technology, Poland
	<b>O.S.III.C.6</b> Distance dependence of MXene-induced fluorescence energy transfer and applications in single-molecule biosensing
	<u>Carmen Lorena Manzanares-Palenzuela<sup>1,2</sup></u> , Dahnan Spurling <sup>3</sup> , Alan Szalai <sup>1,4</sup> , Ece Büber <sup>1</sup> , Tim Schröder <sup>1</sup> , Valeria Nicolosi <sup>3</sup> , Philip Tinnefeld <sup>1</sup>
	<sup>1</sup> Department of Chemistry and Center for NanoScience, Ludwig-Maximilians-University, Munich, Germany, <sup>2</sup> CNRS, Centrale Lille, University Polytechnique Hauts-de-France, UMR 520 - IEMN, LIA LICS, University of Lille, Lille, France, <sup>3</sup> School of Chemistry, Trinity College Dublin, Dublin 2, Ireland, <sup>4</sup> CONICET Centro de Investigaciones en Bionanocien- cias (CIBION), Polo Científico Tecnológico Godoy Cruz, Buenos Aires, Argentina
09 <sup>45</sup> - 10 <sup>00</sup>	O.S.III.C.7 Integration of MXenes in Ceramic Matrices for Enhanced Material Properties
	<u>Maxim Sokol</u> , Barak Ratzker, Or Messer Tel Aviv University, Ramat Aviv, Israel
10 <sup>00</sup> - 10 <sup>15</sup>	<sup>5</sup> O.S.III.C.8
	Utilizing Interferometric Scattering Microscopy to Explore Ion Dynamics within Single Two-Dimensional MXene Nanoparticles
	<u>Mohsen Beladi Mousavi</u> <sup>1</sup> , Franz Gröbmeyer <sup>1</sup> , Christoph Gruber <sup>1</sup> , Kyle Matthews <sup>2</sup> , Kateryna Shevchuk <sup>2</sup> , Alex Inman <sup>2</sup> , John Wang <sup>2</sup> , Yury Gogotsi <sup>2</sup> , Emiliano Cortes <sup>1</sup> <sup>1</sup> Ludwig-Maximilians-Universität München, Faculty of Physics, Munich, Germany, <sup>2</sup> A.J. Drexel Nanomaterials Institute and Department of Materials Science and Engineering, Drexel University, Philadelphia, PA, United States
	T SYMPOSIUM D: ECO-MATERIALS AND ECO-TECHNOLOGIES
10.2 10.2	<b>Photocatalytic coatings with Ce-loaded zeolites</b> Kristina Mojsilović <sup>1</sup> , Srna Stojanović <sup>2</sup> , Maria Serdechnova <sup>3</sup> , Carsten Blawert <sup>3</sup> , Ljiljana Damjanović-Vasilić <sup>2</sup> , Mikhail L. Zheludkevich <sup>3,4</sup> , Stevan Stojadinović <sup>1</sup> ,
	<u>Rastko Vasilić</u> <sup>1</sup> <sup>1</sup> University of Belgrade, Faculty of Physics, Belgrade, Serbia, <sup>2</sup> University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia, <sup>3</sup> Institute of Surface Science,

Faculty of Physical Chemistry, Belgrade, Serbia, <sup>3</sup>Institute of Surface Science, Helmholtz-Zentrum Hereon, Geesthacht, Germany, <sup>4</sup>Institute of Materials Science, Faculty of Engineering, Kiel University, Kiel, Germany

### 10<sup>30</sup> - 10<sup>45</sup> **O.S.III.D.3**

# Effect of plasma treatment on surface chemistry and morphology of jute fibers

<u>Mirjana Kostic</u><sup>1</sup>, Marija Milosevic<sup>1</sup>, Bratislav Obradovic<sup>2</sup>, Matea Korica<sup>3</sup>, Alenka Vesel<sup>4</sup>, Aleksandra Ivanovska<sup>3</sup>, Milorad Kuraica<sup>2</sup>, Zorica Svircev<sup>5,6</sup> <sup>1</sup>Faculty of Technology and Metallurgy, University of Belgrade, Serbia, <sup>2</sup>Faculty of Physics, University of Belgrade, Serbia, <sup>3</sup>Innovation Center of the Faculty of Technology and Metallurgy, University of Belgrade, Serbia, <sup>4</sup>Jožef Stefan Institute, Ljubljana, Slovenia, <sup>5</sup>Faculty of Sciences, University of Novi Sad, Serbia, <sup>6</sup>Faculty of Science and Engineering, Åbo Akademi University, Finland

### 10<sup>45</sup> - 11<sup>00</sup> **O.S.III.D.4**

# Performance Properties of Concrete Produced Using Recycled Polymer Shot

<u>Marcin Małek</u><sup>1</sup>, Katarzyna Jasik<sup>2</sup>, Emil Kardaszuk<sup>1</sup>, Michał Gregorczyk<sup>1</sup>, Waldemar Łasica<sup>1</sup>, Janusz Kluczyński<sup>2</sup>

<sup>1</sup>Military University of Technology, Faculty of Civil Engineering and Geodesy, Testing Laboratory, Warsaw, Poland, <sup>2</sup>Military University of Technology, Faculty of Mechanical Engineering, Institute of Robots & Machine Design, Warsaw, Poland

# 12<sup>00</sup> Awards and Closing of the Conference

12<sup>30</sup> Farewell Cocktail

# ABSTRACTS YUCOMAT Plenary Lectures

# MRS-SERBIA 2024 AWARD FOR A LASTING AND OUTSTANDING CONTRIBUTION TO MATERIALS SCIENCE AND ENGINEERING

### Stimuli-sensitive drug delivery systems

Vladimir Torchilin

Department of Pharmaceutical Sciences and Center for Pharmaceutical Biotechnology and Nanomedicine, Northeastern University, Boston, MA 02115, USA

Drug carriers are used to protect sensitive drug molecules from the inactivation and to improve drug's pharmacokinetics and delivery to the site of disease. Ideally, drug carrier should: (a) accumulate in required organ or tissue, and (b) penetrate inside target cells delivering there its load. Organ or tissue (tumor, infarct) accumulation could be achieved by the passive targeting via the enhanced permeability and retention effect or by the specific ligand(antibody)mediated active targeting, while the intracellular delivery could be mediated by certain internalizable ligands (folate, transferrin) or by cell-penetrating peptides. To be able to behave this way, drug carrier should simultaneously carry on its surface various moieties capable of functioning in a certain orchestrated order. Now, within the frame of this concept, multifunctional stimuli-responsive nanocarriers are developed, i.e. nanocarriers that, depending on the particular requirements, can circulate long; target the site of the disease via both non-specific and/or specific mechanisms; respond local stimuli characteristic of the pathological site by, for example, releasing an entrapped drug or deleting a protective coating facilitating thus the contact between drug-loaded nanocarriers and target cells; and even provide an enhanced intracellular delivery of an entrapped drug with its subsequent delivery to specific intracellular organelles, such as nuclei, lysosomes or mitochondria. Such carriers can be additionally supplemented with reporter moieties to follow their real-time biodistribution and target accumulation. Among new developments to be considered in the area of multifunctional pharmaceutical nanocarriers are: drug- or/and RNA-loaded delivery systems additionally decorated with cell-penetrating peptides for the enhanced intracellular delivery; "smart" multifunctional drug delivery systems, which can reveal/expose temporarily hidden functions under the action of certain local stimuli characteristic for the pathological zone (such as lowered pH, redox-conditions, hypoxia, or locally increased expression of certain enzymes); new means for controlled delivery and release of siRNA; approaches for intracellular drug delivery and organelle targeting; and application of nanocarriers co-loaded with siRNA and drugs to treat multidrug resistant tumors.

### TEM-STEM Studies of Gold Nanoparticles in Twisted MoS<sub>2</sub> Bilayers

<u>Robert Sinclair</u><sup>1</sup>, Yi Cui<sup>1</sup>, Pawel Czaja<sup>1,2</sup> and Yi Cui<sup>1</sup> <sup>1</sup>Department of Materials Science and Engineering, Stanford University, Stanford, CA 94305, United States <sup>2</sup>Institute of Metallurgy and Materials Science, Polish Academy of Sciences, 30-059 Krakow, Poland.

The development of 2D materials such as graphene and metal dichalcogenides has been the subject of much recent research. For possible device applications, their interaction with metal contacts will be critically important. While the epitaxial growth of a pure metal such as FCC gold on hexagonal molybdenum disulfide ( $MoS_2$ ) is well understood, the intercalation of metals between two 2D layers is not, and this could have interesting consequences. Accordingly, we have deposited Au nanoparticles onto thin  $MoS_2$  substrates by electron beam evaporation, applied a second  $MoS_2$  layer with various  $MoS_2$ -MoS<sub>2</sub> twist angles, annealed the samples and examined them by TEM and STEM techniques.

We have found, by through-foil transmission electron microcopy (TEM), that annealing epitaxial gold nanoparticles sandwiched between mechanically twisted MoS<sub>2</sub> bilayers results in morphology changes of the gold into nanodiscs and reorientation of the Au-MoS<sub>2</sub> alignment. At low twist angles, the gold re-orients half-way between the orientation of the encapsulating bilayers, while for larger twists, the re-orientation shows a milder sinusoidal variation with increasing twist ("twisted epitaxy") [1]. This behavior is shown to be consistent with density functional theory (DFT) calculations of the interfacial energies. Application of STEM techniques (e.g. 4D-STEM) allows further analysis of the exact atomic arrangements.

These new findings therefore open up several possibilities for further investigation, in terms of both the systems involved and any influence on physical properties. This paper will discuss progress along these lines.

### **Reference:**

1. Y. Cui *et al.* Science 383 (2024) 212-219

**Acknowledgement**: This work was partly supported by Office of Basic Energy Sciences of the U.S. Department of Energy (DOE), Division of Materials Science and Engineering. Pawel Czaja acknowledges receipt of a Fulbright Fellowship. The authors also appreciate the use and support of the Stanford Nano Shared Facilities (SNSF).

### Synthesis of MXenes by Selective Etching and Chemical Vapor Deposition (CVD)

Yury Gogotsi

A.J. Drexel Nanomaterials Institute and Department of Materials Science and Engineering, Drexel University, Philadelphia, PA 19104, USA

MXenes are potentially the largest family of 2D materials with diverse properties. They have a general chemical formula of  $M_{n+1}X_nT_x$ , where M represents a transition metal (Ti, Mo, Nb, V, Cr, *etc.*), X is either carbon and/or nitrogen (n=1, 2, 3 or 4), and  $T_x$  stands for surface terminations (O, OH, halogens, chalcogens, *etc.*) [1]. More than 100 stoichiometric  $M_{n+1}X_n$  structures (not including surface terminations) have been predicted. Availability of solid solutions on the M site (including high-entropy MXenes) and X site (carbonitrides and oxycarbides) and control of surface terminations, create an opportunity for the atomistic design of numerous new structures and compositions. More than 40 stoichiometric MXenes and dozens of solid solutions and MXenes with various terminations have been reported.

In the past years, a major progress has been achieved in synthesis of MXenes, with wet chemical selective etching of MAX phases being supplemented by electrochemical etching, etching in Lewis acid molten salts, extraction of A element by gaseous halogens and CVD synthesis from inexpensive precursors such as titanium chlorides and natural gas [1-4]. Some of those methods offer a cleaner and less expensive alternative to HF etching [3]. Even more important, materials produced using different methods have different properties. For example, MXenes from etching in acidic solutions are hydrophilic due to mixed O and OH terminations, while the same  $M_{n+1}X_n$  MXenes with CI terminations resulting from the molten salt etching are hydrophobic [4]. The surface composition allows one to control properties of MXenes and tune their electronic conductivity, optical, electrochemical and mechanical properties.

- 1. K. R. G. Lim, M. Shekhirev, B. C. Wyatt, B. Anasori, Y. Gogotsi, Z. W. Seh, Fundamentals of MXene synthesis, *Nature Synthesis*, 1 (8) 601-614 (2022)
- 2. M. Downes, C. E. Shuck, J. McBride, J. Busa, Y. Gogotsi, Comprehensive Synthesis of Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> from MAX phase to MXene, *Nature Protocols*, **19**, 1807–1834 (2024)
- 3. E. Rems, M. Anayee, E. Fajardo, R. L. Lord, D. Bugallo, Y. Gogotsi, Y.-J. Hu, Computationally guided synthesis of MXenes by dry selective extraction, *Advanced Materials*, **35**, 2305200 (2023)
- 4. T. Zhang, K. Shevchuk, R. (John) Wang, J. AlHourani, H. Kim, Y. Gogotsi, Delamination of chlorine-terminated MXene produced using molten salt etching, *Chemistry of Materials*, **36** (4) 1998–2006 (2024)

#### 25<sup>th</sup> YUCOMAT 2024 & XIII WRTCS Herceg Novi, September 2 - 6, 2024

### Y.PL.S.I.3

## Colloidal nanomaterials for light

Andrey L. Rogach Department of Materials Science and Engineering & Centre for Functional Photonics, City University of Hona Kona, Hona Kona S.A.R.

I will provide an overview on synthesis, optical spectroscopy, and applications of light-emitting colloidal nanomaterials recently (2022-2024) synthesized in our labs, which include CuInSebased [1] and HgTe nanorods [2] emitting over the broad visible and infrared spectral range, carbon dots [3], and perovskite nanocrystals [4]. I will highlight their photophysical properties studied by advanced optical spectroscopy techniques, and demonstrate their applications in light-emitting diodes [3,5,6] and photodetectors [2,7].

- Portniagin, A.S.; Ning, J.; Wang, S.; Li, Z.; Sergeev, A.A.; Kershaw, S.V.; Zhong, X.; Rogach, A.L. Monodisperse CuInS<sub>2</sub>/CdS and CuInZnS<sub>2</sub>/CdS Core-Shell Nanorods with a Strong Near-Infrared Emission. *Adv. Opt. Mater.* 2022, 10, 2102590.
- 2. Portniagin, A.S.; Sergeeva, K.A.; Kershaw, S.V.; Rogach, A.L. Cation-Exchange-Derived Wurtzite HgTe Nanorods for Sensitive Photodetection in the Short-Wavelength Infrared Range. *Chem. Mater.* **2023**, *35*, 5631–5639.
- Cherevkov, S.A.; Stepanidenko, E.A.; Miruschenko, M.D.; Zverkov, A.M.; Mitroshin, A.M.; Margaryan, I.V.; Spiridonov, I.G.; Danilov, D.V.; Koroleva, A.V.; Zhizhin, E.V.; Baidakova, M.V.; Sokolov, R.V.; Sandzhieva, M.A.; Ushakova, E.V.; Rogach, A.L. Amphiphilic Acetylacetone-Based Carbon Dots. J. Mater. Chem. C 2024, 12, 3943–3952.
- 4. Zeng, Q.; Zhang, X.; Bing, Q.; Xiong, Y.; Yang, F.; Liu, H.; Liu, J.-Y.; Zhang, H.; Zheng, W.; Rogach, A.L.; Yang, B. Surface Stabilization of Colloidal Perovskite Nanocrystals via Multi-Amine Chelating Ligands. ACS Energy Lett. **2022**, *7*, 1963–1970.
- Dong, W.; Zhang, X.; Yang, F.; Zeng, Q.; Yin, W.; Zhang, W.; Wang, H.; Yang, X.; Kershaw, S.V.; Yang, B.; Rogach, A.L.; Zheng, W. Amine-Terminated Carbon Dots Linking Hole Transport Layer and Vertically Oriented Quasi-2D Perovskites through Hydrogen Bonds Enable Efficient LEDs. ACS Nano 2022, 16, 9679–9690.
- Guo, J.; Lu, M.; Zhang, X.; Sun, S.; Han, C.; Zhang, Y.; Yang, X.; Kershaw, S.V.; Zheng, W.; Rogach, A.L. Highly Stable and Efficient Light-Emitting Diodes Based on Orthorhombic γ-CsPbI3 Nanocrystals. ACS Nano 2023, 17, 9290–9301.
- Sergeeva, K.A.; Hu, S.; Sokolova, A.V.; Portniagin, A.S.; Chen, D.; Kershaw, S.V.; Rogach, A.L. Obviating Ligand Exchange Preserves the Intact Surface of HgTe Colloidal Quantum Dots and Enhances Performance of Short Wavelength Infrared Photodetectors. *Adv. Mater.* 2024, 36, 2306518.

# From aerosol synthesis of materials and devices to a new value for the mean free path of air

Sotiris E. Pratsinis

#### Particle Technology Laboratory, ETH Zürich, Sonneggstrasse 3, CH-8092 Zürich, Switzerland

Recent advances in understanding of combustion and aerosol formation and growth through multiscale process design, allow now inexpensive synthesis of nanoparticles with sophisticated composition, size and morphology by flame spray combustion at kg/h even at an academic institution with such units now all over the world (UK, Spain, India etc.). These have led to synthesis of single noble atom heterogeneous catalysts, biomaterials and highly porous sensing films that led to commercial devices for detection of adulterated liquor that are sold today all over the planet.

These advances and community's keen interest on nanoscale phenomena have motivated a closer look to the fundamentals of aerosol dynamics in the free molecule regime. The mean free path (MFP) dictates when gas-phase nanoparticle transport takes place in the free molecule or continuum regime. This distinction is crucial in process design of gas phase processes (laser, plasma, hot wall, ultrasonic and flame) in synthesis of films and nanoparticles especially at the lowest end of nano to sub-nano scale.

For eons, the kinetic theory of gases has been used to determine the MFP assuming elastic collisions between spherical gas molecules [1]. However, is this so with what we know about molecular shape and force fields today? Having reached a state of maturity now, molecular dynamics (MD) simulations can elucidate the fundamentals of basic gas-phase (aerosol) processes that lead to better understanding of natural phenomena and accelerating process scale-up [2]. Here the mechanics of gas collisions are elucidated for plain air at room temperature by thoroughly-validated atomistic MD treating  $O_2$  and  $N_2$  as true diatomic molecules accounting for their shape and force field, for the first time to our knowledge. So it is revealed that their trajectories are no longer straight, and collision frequencies were much higher due to the attractive part of the force field and the diatomic, thus more voluminous, shape of  $N_2$  and  $O_2$  as will be shown by the respective videos. Detailed analysis of the latter trajectories revealed that molecular collisions involve strong interactions between colliding molecules. Frequently, colliding molecules were split from each other but soon return to collide again and again without interacting with any other molecule in between resulting in orbiting collisions as had been envisioned 70 years ago [3]. A direct result of the enhanced interactions between air molecules when treated as true diatomic molecules is that their MFP comes out to be considerably smaller than that from the classic kinetic theory. The new MFP for air is 38.5 nm, almost 43 % smaller than that in textbooks of 67.3 nm at 300 K & 1 atm [4]. Aside from its fundamental value, such a result is significant in gas-phase synthesis of tiny (< 5 nm) nanoparticles where asymptotic (self-preserving) particle size distributions and (fractal-like) structure have not been attained yet to simplify the corresponding process design.

- 1. Maxwell JCMA, The London, Edinburgh, Dublin Philos. Mag. J. Sci., 19-32 (1860).
- 2. Mavrantzas VG & Pratsinis SE, Curr. Opinion Chem. Eng., 23 174 183 (2019).
- 3. Hirschfelder, JO, Curtiss, CF, Bird, RB, Molecular Theory of Gases & Liquids, Wiley, 1954.
- 4. Tsalikis D, Mavrantzas VG, Pratsinis SE, Aerosol Sci. Technol. in press (2024).

### Probing the Ion Flux at the Nanoscale with Operando Technologies

Kangkang Ge<sup>1</sup>, Jeronimo Miranda-Castro<sup>1</sup>, Audrey Perju<sup>1</sup>, B. Mondal<sup>1</sup>, Pierre-Louis Taberna<sup>1</sup>, <u>Patrice Simon<sup>1,2</sup></u> <sup>1</sup>Université Paul Sabatier, CIRIMAT UMR CNRS 5085, 118 Route de Narbonne, 31062 Toulouse, France

<sup>2</sup>Réseau sur le Stockage Electrochimique de l'Energie (RS2E), FR CNRS 3459, France

Understanding local electrochemical processes in energy storage electrodes is crucial for designing efficient materials for batteries and supercapacitors. This underscores the pivotal role of advanced electrochemical characterization techniques, which will be illustrated through several examples.

Firstly, Electrochemical Quartz Crystal Microbalance (EQCM) and Electrochemical Dilatometry (ECD) techniques were employed to track ion fluxes during cation insertion in 2D materials such as  $TiS_2$ , MXene, and rGO [1-3]. The results highlight the key role of electrolyte-material interactions and suggest that the observed improvements in electrochemical performance could be attributed to partial desolvation of electrolyte ions due to their confinement in interlayer spacing [3,4].

In the final part, we will introduce a novel in-plane electrochemical impedance spectroscopy technique used to deconvolute the ionic and electronic contributions in LiFePO<sub>4</sub> and  $Na_3V_2(PO_4)_3F_2$  electrodes during operation [5]. This innovative setup provides a new tool to further evaluate and enhance the performance of electrode materials for energy storage devices by offering new insights into the electronic and ionic transport mechanisms in electrodes during operation.

- 1. K. Ge, H. Shao, E. Raymundo-Piñero, P.-L. Taberna & P. Simon, Nature Communications 15, 1935 (2024).
- 2. J. Miranda-Castro, G. Franklin, T. S. Mathis, P.L. Taberna, P. Simon, Energy Storage Materials, 65, (2024), 103105
- 3. L. Liu, E. Raymundo-Piñero, P.-L. Taberna and P. Simon, Angew. Chem. Int. Ed. 2024.
- 4. S. Fleischmann et al., Nature Energy 2022.
- 5. V. Maurel, K. Brousse, T. S. Mathis, A. Perju, P.L. Taberna and P. Simon, Journal of The Electrochemical Society, 169, 12, 2022, 120510.

### X-ray microscopy at electrochemical systems for sustainable energy technologies

Ehrenfried Zschech Brandenburg University of Technology Cottbus-Senftenberg, Cottbus, Germany

The development of new materials for efficient and durable systems used for sustainable energy technologies is crucial for current and future energy technologies. Performance and lifetime of these electrochemical systems depend on the 3D morphology of the materials and on morphology changes during operation. A profound understanding of degradation mechanisms that affect the performance and limit the lifetime of systems for energy storage and conversation is mandatory for more stable and robust solutions.

High-resolution X-ray imaging provides nondestructive characterization capabilities on opaque objects, observing features with sizes across a range of length scales, down to several 10 nanometers using lens-based full-field X-ray microscopy (TXM). Multi-scale X-ray computed tomography (XCT), characterized by a sample thickness / resolution value of  $\sim 10^3$ , and subsequent 3D data reconstruction is an efficient approach to study the 3D morphology of hierarchically structured systems and materials. Laboratory TXM and nano-XCT provide highresolution 3D information about the morphology of materials for battery electrodes and electrocatalytic systems for water splitting. In an in-situ study, the 3D morphology of Na0.9Fe0.45Ti1.55O4 sodium iron titanate cathode material in Li-ion batteries and microcracks are imaged with sub-100nm resolution. The size- and density-dependence of the fracture behavior of the cathode-material particles is revealed based on a semi-quantitative analysis of the formation and propagation of microcracks in particles [1]. Multi-scale X-ray imaging of a novel transition-metal-based electrocatalytic system for water splitting provides 3D information of the morphology of the hierarchical MoNi<sub>4</sub>/MoO<sub>2</sub>@Ni structure - MoNi<sub>4</sub> electrocatalysts anchored on  $MoO_2$  cuboids aligned on Ni foam – a material system with high electrocatalytic efficiency for hydrogen evolution reaction. MicroXCT images clearly resolve the Ni foam and the attached needle-like  $MoO_2$  micro cuboids. Laboratory nano-XCT shows that the  $MoO_2$  micro cuboids are vertically arranged on Ni foam. MoNi<sub>4</sub> nanoparticles with a size of 20 to 100 nm, positioned on single  $MoO_2$  cuboids, were imaged using SR nano-XCT [2].

- 1. V Shapovalov et al., Crystals 12 (1), 3 (2022)
- 2. E. Zschech et al., Micron 158, 103262 (2022)

### Creation and Characterization of Nanopores in Hexagonal Boron Nitride via Aberration-Corrected Scanning Transmission Electron Microscopy

Rachael Keneipp<sup>1</sup>, Pia Bhatia<sup>1</sup>, Jordan Gusdorff<sup>2,3</sup>, Lee Bassett<sup>3</sup>, <u>Marija Drndić<sup>1</sup></u> <sup>1</sup>Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, PA, USA, <sup>2</sup>Department of Material Science and Engineering, University of Pennsylvania, Philadelphia, PA, USA, <sup>3</sup>Department of Electrical and Systems Engineering, University of Pennsylvania, Philadelphia, PA, USA

The discovery of room-temperature single photon emission (SPE) in hexagonal boron nitride (hBN) launched it to the forefront of research as a promising platform for room-temperature quantum optics and photonics. Room-temperature quantum emission centers in hBN exhibit single-photon emission and optically addressable spin states, as desired for many quantum technologies. In this work, we create and characterize nanopores in hexagonal boron nitride (hBN) via aberration corrected scanning transmission electron microscopy (AC-STEM) drilling and photoluminescent (PL) spectroscopy. Using a finely tuned electron beam, defects on the sub-nanometer to nanometer scale are induced in hBN through electron irradiation and AC-STEM drilling. Atomic-resolution electron energy loss spectroscopy (EELS) is used to monitor and characterize the generation of these defects in real time, and atomic AC-STEM imaging is used to understand the atomic structure of the defects. Confocal PL spectroscopy is subsequently employed to characterize the optical activity of the defects created through electron irradiation and drilling. Through this work, we demonstrate the proof of principle to create defects in hBN of desired size, shape, and location. This work paves the way for controllable defect engineering in hBN and other 2D materials through AC-STEM drilling.

#### **Exploration of New 2D Materials and Their New Properties**

Hui-Ming Cheng

Institute of Technology for Carbon Neutrality, Shenzhen Institute of Advanced Technology, Chinese Academy of Sciences, Shenzhen, China; Faculty of Materials Science and Energy Engineering, Shenzhen University of Advanced Technology, Shenzhen, China and Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, Shenyang, China

Identification of two-dimensional (2D) materials in the monolaver limit has led to discoveries of new phenomena and unusual properties. In this lecture, I'll first report the growth of largearea high-quality 2D ultrathin Mo<sub>2</sub>C crystals by CVD [1], which show 2D characteristics of superconducting transitions that are consistent with Berezinskii–Kosterlitz–Thouless behaviour and show strong dependence of the superconductivity on the crystal thickness. Furthermore, when we introduce elemental silicon during CVD growth of nonlayered molybdenum nitride, we have grown centimeter-scale monolayer films of MoSi<sub>2</sub>N<sub>4</sub> which does not exist in nature and exhibits semiconducting behavior, high strength, and excellent ambient stability [2]. On the other hand, we have found some interesting properties from well-known 2D materials such as h-BN. For example, a class of membranes assembled with 2D transitionmetal phosphorus trichalcogenide nanosheets give exceptionally high ion conductivity and superhigh lithium ion conductivity [3]. We even demonstrate an anomalously large magnetobirefringence effect in transparent suspension of magnetic 2D crystals [4], with orders of magnitude larger than that in previously known transparent materials. Moreover, based on this phenomenon, we develop a stable and birefringence-tunable deep-ultraviolet modulator from 2D hexagonal boron nitride which gives rise to a ultra-high specific magneto-optical Cotton-Mouton coefficient, about five orders of magnitude higher than other potential deepultraviolet-transparent media [5]. Very recently, we have found that strong bulk van der Waals materials can be densified from their nanosheets at near room temperatures with mediation of water [6]. These findings indicate a great promise of 2D materials.

- Xu, C.; Wang, L.; Liu, Z.; Chen, L.; Guo, J.; Kang, N.; Ma, X.-L.; Cheng, H.-M.; Ren, W. Large-Area High-Quality 2D Ultrathin Mo2C Superconducting Crystals. *Nat. Mater.* 2015, 14, 1135– 1141.
- 2. Hong, Y.L.; Liu, Z.; Wang, L.; Zhou, T.; Ma, W.; Xu, C.; Feng, S.; Chen, L.; Chen, M.L.; Sun, D.M.; et al. Chemical vapor deposition of layered two-dimensional MoSi2N4 materials. *Science* **2020**, *369*, 670–674.
- Qian, X.; Chen, L.; Yin, L.; Liu, Z.; Pei, S.; Li, F.; Hou, G.; Chen, S.; Song, L.; Thebo, K.H.; et al. CdPS3 nanosheets-based membrane with high proton conductivity enabled by Cd vacancies. *Science* 2020, 370, 596–600.
- 4. Ding, B.; Kuang, W.; Pan, Y.; Grigorieva, I.V.; Geim, A.K.; Liu, B.; Cheng, H.M. Giant magnetobirefringence effect and tuneable colouration of 2D crystal suspensions. *Nat. Commun.* **2020**, *11*, 3725.
- 5. Xu, H.; Ding, B.; Xu, Y.; Huang, Z.; Wei, D.; Chen, S.; Lan, T.; Pan, Y.; Cheng, H.M.; Liu, B. Magnetically tunable and stable deep-ultraviolet birefringent optics using two-dimensional hexagonal boron nitride. *Nat. Nanotechnol.* **2022**, *17*, 1091–1096.
- 6. Zhu, J.; Li, F.; Hou, Y.; Li, H.; Xu, D.; Tan, J.; Du, J.; Wang, S.; Liu, Z.; Wu, H.; Wang, F.; Su, Y.; Cheng, H.M. Near-room-temperature water-mediated densification of bulk van der Waals materials from their nanosheets. *Nat. Mater.* **2024**, *23*, 604–611.

### Beyond Layers: Unveiling the Potential of Organic 2D Crystals in Emerging Material Science

Xinliang Feng Max Planck Institute of Microstructure Physics, Halle (Saale), Germany and Technische Universität Dresden, Dresden, Germany

Organic 2D crystals with extended in-plane conjugation and strong interlayer coupling have emerged as a distinctive class of layered materials characterized by unique electronic structures and exotic physicochemical phenomena, with significant application potential. A widely employed approach for synthetic access to these precision materials is bottom-up synthesis. This encompasses the creation of single-layer to few-layer 2D polymers/supramolecular polymers, 2D conjugated polymers or covalent-organic frameworks, and 2D conjugated metalorganic frameworks. A key chemical challenge is to achieve controlled 2D polymerization in two distinctive directions under thermodynamic/kinetic control in solution, in the solid state, or at the surface/interface. In the first part of my talk, I will present novel 2D polymerization methods together with design strategies aimed at achieving efficient 2D conjugation in specific 2D conjugated polymers, such as 2D poly(arylenevinylene)s and 2D poly(benzimidazobenzophenanthroline)-ladder-type structures. These 2D conjugated polymers provide a material platform for realizing high intrinsic carrier mobilities, which is crucial for future organic optoelectronics and spintronics. In the next part, I will present our recent progress in 2D conjugated metal-organic framework materials, highlighting their applications in MOFtronics and beyond. In the following part, I will discuss on-water surface chemistry as a potent synthetic platform for organic 2D crystals and their van der Waals heterostructures, leveraging water-surface confinement and enhanced chemical reactivity and selectivity. A major focus will be on the surfactant-monolayer-assisted interfacial synthesis (SMAIS) method, which is now known for its high efficiency in the programmable arrangement of precursor monomers on the water surface and subsequent controlled 1D/2D polymerization. The distinct 2D crystal structures that offer tailorable conjugated building blocks and conjugation lengths, tunable pore sizes and thicknesses, and remarkable electronic structures, make these materials highly promising for various applications in electronics, optoelectronics, and spintronics. Other physicochemical phenomena and application potential of organic 2D crystals, such as in membranes and emergent energy devices, will also be discussed.

#### Low-Dimensional Neuromorphic Electronic Materials and Applications

Mark C. Hersam

Department of Materials Science and Engineering, Northwestern University, 2220 Campus Drive, Evanston, IL 60208-3108, USA

The exponentially improving performance of digital computers has recently slowed due to the speed and power consumption issues resulting from the von Neumann bottleneck. In contrast, neuromorphic computing aims to circumvent these limitations by spatially co-locating logic and memory in a manner analogous to biological neuronal networks [1]. Beyond reducing power consumption, neuromorphic devices provide efficient architectures for image recognition. machine learning, and artificial intelligence [2]. This talk will explore how low-dimensional nanoelectronic materials enable gate-tunable neuromorphic devices [3]. For example, by utilizing self-aligned, atomically thin heterojunctions, dual-gated Gaussian transistors have been realized, which show tunable anti-ambipolarity for artificial neurons, competitive learning, spiking circuits, and mixed-kernel support vector machines [4,5]. In addition, fielddriven defect motion in polycrystalline monolayer MoS<sub>2</sub> enables gate-tunable memristive phenomena that serve as the basis of hybrid memristor/transistor devices (*i.e.* 'memtransistors') that concurrently provide logic and data storage functions [6]. The planar geometry of memtransistors further allows multiple contacts and dual gating that mimic the behavior of biological systems such as heterosynaptic responses [7]. Moreover, control over polycrystalline grain structure enhances the tunability of potentiation and depression, which enables unsupervised continuous learning in spiking neural networks [8]. Finally, the moiré potential in asymmetric twisted bilayer graphene/hexagonal boron nitride heterostructures gives rise to robust electronic ratchet states. The resulting hysteretic, non-volatile injection of charge carriers enables room-temperature operation of moiré synaptic transistors with diverse biorealistic neuromorphic functionalities and efficient compute-in-memory designs for low-power artificial intelligence and machine learning hardware [9].

- 1. Sangwan, V.K.; Liu, S.E.; Trivedi, A.R.; Hersam, M.C. Two-Dimensional Materials for Bio-Realistic Neuronal Computing Networks. *Matter* **2022**, *5*, 4133–4152.
- 2. Sangwan, V.K.; Hersam, M.C. Neuromorphic nanoelectronic materials. *Nat. Nanotechnol.* **2020**, *15*, 517–528.
- 3. Beck, M.E.; Hersam, M.C. Emerging Opportunities for Electrostatic Control in Atomically Thin Devices. *ACS Nano* **2020**, *14*, 6498–6518.
- 4. Beck, M.E.; Shylendra, A.; Sangwan, V.K.; Guo, S.; Rojas, W.A.G.; Yoo, H.; et al. Spiking neurons from tunable Gaussian heterojunction transistors. *Nat. Commun.* **2020**, *11*, 1565.
- Yan, X.; Qian, J.H.; Ma, J.; Zhang, A.; Liu, S.E.; Bland, M.P.; et al. Reconfigurable mixed-kernel heterojunction transistors for personalized support vector machine classification. *Nat. Electron.* 2023, 6, 862–869.
- 6. Yan, X.; Qian, J.H.; Sangwan, V.K.; Hersam, M.C. Progress and challenges for memtransistors in neuromorphic circuits and systems. *Adv. Mater.* **2022**, *34*, 2108025.
- 7. Lee, H.S.; Sangwan, V.K.; Rojas, W.A.G.; Bergeron, H.; Jeong, H.Y.; Yuan, J.; *et al.* Dual-gated MoS<sub>2</sub> memtransistor crossbar array. *Adv. Funct. Mater.* **2020**, *30*, 2003683.
- Yuan, J.; Liu, S.E.; Shylendra, A.; Rojas, W.A.G.; Guo, S.; et al. Reconfigurable MoS<sub>2</sub> memtransistors for continuous learning in spiking neural networks. *Nano Lett.* 2021, 21, 6432-6440.
- 9. Yan, X.; Zheng, Z.; Sangwan, V.K.; Qian, J.H.; Wang, X.; Liu, S.E.; et al. Moiré synaptic transistor with room-temperature neuromorphic functionality. *Nature* **2023**, *624*, 551–556.

# Y.PL.S.III.11 Imaging of short range order with electron microscopy: from high performance alloys to semiconductor thin films

Andrew M. Minor

Department of Materials Science and Engineering, University of California, Berkeley, CA, 94720 USA and the National Center for Electron Microscopy, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA, 94720 USA

This talk will describe our recent results utilizing energy filtered diffraction, 4D-STEM and in situ TEM nanomechanical testing that provide insight into the determination and role of short range order (SRO) in materials. Examples will be presented from structural alloys such as  $\alpha$ -titanium and the CrCoNi medium entropy alloy, as well as semiconductors such as a SiGeSn/GeSn multilayer. We will consider the role of both SRO and planar defects in the both the mechanical response as well as structural determination via electron diffraction as a function of heat treatment in the CrCoNi MEA. Lastly, we will discuss both the strengths and limitations of TEM methods for analyzing SRO in these systems, with particular emphasis on coordinated computational methods to simulate diffraction patterns in order to directly compare with experimental measurements.

### **Sponsor lecture**

### U.S. Air force office of scientific research grant funding opportunities

David Swanson

### U.S. Air Force Office of Scientific Research, European Office of Aerospace Research and Development

This presentation will highlight various opportunities for research grant funding, which is available each year through the U.S. Air Force Office of Scientific Research (AFOSR). The European Office of Aerospace Research and Development (EOARD) is one of the international locations of AFOSR, and it is in London in the United Kingdom. This European grant funding office is made up of scientists and engineers who review research topic ideas and make decisions on the best distribution of grant funding for qualified researchers and professors at any European universities. This presenter is responsible for funding programs within the material science and structures topic areas. This presentation will provide an overview of AFOSR and EOARD, as well as give detailed instructions on how professors or post-doctoral researchers from any university throughout Europe may inquire about and apply for grant funding opportunities. EOARD provides grants for in-house university research programs, as well as conference support, and visiting scientist travel costs to collaborate in the U.S.A. Many researchers within universities in nearly every country in Europe are currently supported by the U.S. Air Force. EOARD seeks to financially support innovative basic science that will benefit the aerospace community at large.

# YUCOMAT Oral Presentations

### O.S.I.B.1

### Halogen Bonding: A Pathway to More Stable Perovskite Solar Cells

Jovan Lukić<sup>1,2</sup>, Vuk V. Radmilović<sup>1</sup>, Jovana V. Milić<sup>2</sup> <sup>1</sup>Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia <sup>2</sup>Adolphe Merkle Institute, University of Fribourg, Fribourg, Switzerland

Hybrid metal halide perovskites have shown potential in photovoltaics over the last decade [1,2]. Despite high solar-to-electric power conversion efficiencies and excellent optoelectronic properties, these materials are hindered by stability issues caused by operating conditions [3]. One of the leading sources of instabilities occurs at the interfaces with the charge transport layers and is caused by ion migration [2]. There have been efforts to address this by relying on interfacial engineering, such as using supramolecular modulators featuring halogen bonding (XB) [4]. Metal oxides, as the most frequently used charge-transport layers for hybrid perovskite solar cells, are suitable for XB as a way to improve operational stability [3]. XB can affect hydrophobicity, ion migration, and charge transfer, affecting the resulting photovoltaic characteristics [5]. We applied 1.4-dijodotetrafluorobenzene (TFDIB) as an XB agent at the interface of  $TiO_2$  in perovskite solar cells [6]. We investigate structural and optoelectronic characteristics by a combination of techniques, including scanning electron microscopy, X-ray diffraction, UV-vis absorption, photoluminescence spectroscopy, X-ray and ultraviolet photoelectron spectroscopy, to identify interfacial changes upon XB modulation [6]. As a result, we demonstrate the improvement of operational stability in perovskite solar cells, providing a versatile supramolecular strategy in hybrid photovoltaics.

- 1. A. K. Jena, A. Kulkarni and T. Miyasaka, Chem. Rev., 2019, 119, 3036–3103.
- 2. J. V. Milić, J. Mater. Chem. C, 2021, 9, 11428-11443.
- 3. M. L. Ball, J. V. Milić and Y.-L. Loo, Chem. Mater., 2022, 34, 2495-2502.
- 4. L. Canil, J. Salunke, Q. Wang, M. Liu, H. Köbler, M. Flatken, L. Gregori, D. Meggiolaro, D. Ricciarelli, F. De Angelis, M. Stolterfoht, D. Neher, A. Priimagi, P. Vivo and A. Abate, *Advanced Energy Materials*, 2021, **11**, 2101553.
- 5. M. A. Ruiz-Preciado, D. J. Kubicki, A. Hofstetter, L. McGovern, M. H. Futscher, A. Ummadisingu, R. Gershoni-Poranne, S. M. Zakeeruddin, B. Ehrler, L. Emsley, J. V. Milić and M. Grätzel, J. Am. Chem. Soc., 2020, **142**, 1645–1654.
- 6. J. Lukic, G. Bravetti, J. A. Venegas, P. Zimmermann, T.-D. Nguyen, A. Hinderhoffer, F. Schreiber, A. Sastre-Santos, J.-Y. Seo, V. V. Radmilović and J. V. Milić, 2024, manuscript in preparation.

### O.S.I.B.2

# Enhancing water splitting efficiency through structural and chemical modifications of cellulose-derived electrocatalysts based on nickel phosphides

Klaudia Maślana, Karolina Pietrusewicz, Ewa Mijowska

West Pomeranian University of Technology, Szczecin, Faculty of Chemical Technology and Engineering, Department of Nanomaterials Physicochemistry, Piastow Ave. 45, 70-311 Szczecin, Poland

The urgent global need for sustainable energy has intensified research into green resources, with water splitting emerging as a promising avenue for electricity generation. Electrochemical water splitting involves hydrogen evolution reaction (HER) and oxygen evolution reaction (OER), with OER being the more energy-consuming with a sluggish kinetic step.

In this study, cellulose-derived electrocatalysts, particularly focusing on nickel phosphides  $(Ni_xP_y)$  functionalized cellulose platforms, as efficient catalysts for OER have been explored. Carbonized and activated cellulose fibers served as a substrate for depositing  $Ni_xP_y$  nanoparticles. Additionally, systematic research has been undertaken to assess the impact of transition metal doping (Mn, Fe, Ni) and structural modifications for electrocatalytic properties. These findings are supported by a range of physicochemical analyses (such as TEM, XRD, XPS, and AAS).

The resultant electrocatalysts demonstrate enhanced performance owing to uniform  $Ni_xP_y$  coverage and the high surface area of the carbon platform. Various tests, including linear sweep voltammetry (LSV), electrochemical impedance spectroscopy (EIS), Tafel analysis, and stability tests have been conducted to determine electrochemical activity. When compared to commercial RuO<sub>2</sub> and Pt/C, which are considered perfect reference catalysts, the prepared materials exhibit comparable or even superior properties. For instance, the overpotential value for cel\_Ni<sub>2</sub>P\_+10%Ni has decreased by 64 mV in OER compared to RuO<sub>2</sub>, and the Tafel slope value has decreased by approximately ~45%.

Our study offers a cost-effective and sustainable alternative to coal-based energy generation by utilizing cellulose-derived electrocatalysts and nickel phosphides, potentially replacing noble metals and contributing to the development of environmentally friendly water-splitting technologies.

#### O.S.I.B.3

#### Cost-Efficient Method for Deterministic Creation of Single Photon Emitters in GaSe

<u>Sanja Đurđić Mijin</u><sup>1,2</sup>, Ismael dePedro-Embid<sup>3</sup>, Snežana Lazić<sup>1,4,5</sup> <sup>1</sup>Departamento de Fisica de Materiales, Facultad de Ciencias, Universidad Autonoma de Madrid (UAM), 28049 Madrid, Spain

<sup>2</sup>Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia <sup>3</sup>Paul-Drude-Institut fur Festkorperelektronik, Leibniz- Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5–7, 10117 Berlin, Germany

<sup>4</sup>Instituto Universitario de Ciencia de Materiales "Nicolas Cabrera" (INC, UAM, 28049 Madrid, Spain <sup>5</sup>Condensed Matter Physics Center (IFIMAC), UAM, 28049 Madrid, Spain

The ever-increasing knowledge in the field of quantum technology led to its applicability in nonlaboratory environments such as economy, industry and everyday life. Through continued research and development, we inch closer to realizing the full potential of quantum technologies, promising a future that transcends the limitations of the present digital era. At the core of this research are single photon emitters (SPEs), foundational quantum light resources that hold immense promise for scalable quantum technologies including quantum computing. cryptography, communication, and sensing. Achieving a single-photon source that is both stable and scalable is not just a challenge, but it is also crucial for the widespread adoption of quantum technologies in real-world applications. Among various available non-classical light sources, localized defect states in two-dimensional (2D) van der Waals (vdW) materials have emerged as a promising physical system for scalable quantum technologies due to their tunable bandgaps, layer-dependent excitonic properties, and efficient charge carrier confinement. 2D SPEs offer high brightness and purity, spectral tenability, high photon extraction efficiency, and can operate under ambient conditions. Moreover, it is demonstrated that the confinement potentials of carriers in semiconducting 2D materials can be systematically tailored through localized adjustments of the bandgap via electrostatic or strain field modulation. Here, we report a costefficient and practical methodology for the precise placement of single-photon emitters (SPEs) within GaSe flakes through strain engineering utilizing optically active microparticles with a distinctive bipyramidal shape. The bipyramidal shape enhances strain-induced effects crucial for single-photon emitter creation, whereas the optical activity of the particles allows precise identification of their position via conventional optical spectroscopy measurements, eliminating the need for SEM or AFM. Using the presented method, we successfully generated localized SPEs in a thin GaSe flake, producing exciton-biexciton cascades with elliptically polarized emission. The detection of excitonic complexes in locally engineered traps within GaSe sheets indicates the system's potential for producing entangled photon pairs through an XX-X radiative cascade. This holds particular significance, considering that externally applied strain and/or electric field can also control the polarization state of the emitted X-XX cascade.

The excellent agreement between our results and prior reports on strain-induced SPEs in GaSe undeniably affirms the suitability of our method for the precise creation of highly localized SPEs. The introduction of this cost-effective and practical platform for quantum emitter generation expands the accessibility of 2D SPEs, fostering advancements in both research and practical applications in the field. Altogether, our study demonstrates a pioneering cost-efficient approach for intentionally generating site- and size-controlled single photon emitters in 2D materials through strain engineering. The implementation of this practical and economically viable technique for quantum emitter generation expands the accessibility of 2D SPEs, thereby facilitating progress in both academic research and real-world applications within the field.

### 0.S.I.C.1

### Progress in Bubble-Printing: Fabrication of Ti<sub>3</sub>C<sub>2</sub>T<sub>X</sub> MXene Strain Sensors

Marcel Herber, Eric H. Hill

Institute of Physical Chemistry, University of Hamburg, 20146 Hamburg, Germany and The Hamburg Center for Ultrafast Imaging (CUI), 22761 Hamburg, Germany

MXenes, which have recently been included in the family of 2D materials, have remarkable properties such as high conductivity, plasmonic properties and resistance to high temperatures. These properties have led to their use in various fields such as energy storage, electronics, and sensor technology. While conventional methods such as inkjet printing, screen printing, and 3D extrusion are commonly used to print MXenes, the use of optically directed techniques has not yet been established.

The optical control of microbubbles offers a novel approach for the assembly of colloidal particles on surfaces. A microbubble is formed at the interface between the substrate and the colloidal suspension, attracting the particles due to Marangoni convection and immobilizing them on the surface through van der Waals interactions. Recent studies have investigated the effects of various parameters such as surface chemistry, solvent composition, MXene concentration and laser intensity on the bubble printing of MXenes. These findings allowed successful bubble printing of a colloidal dispersion of MXene nanosheets on a non-plasmonic substrate without affecting their conductivity and plasmonic properties.

In this study, bubble printing was used to bubble-print a composite of MXene nanosheets and the conductive polymer PEDOT:PSS onto a flexible substrate to fabricate strain sensors. This study investigates not only the assembly of MXene nanosheets with PEDOT:PSS, but also how the different amounts of polymer affect the properties of the strain sensors in terms of durability and sensitivity.

### 0.S.I.C.2

## TM<sub>1/3</sub>TaS<sub>2</sub>-based Transition Metal Compound Catalysts: Driving Forward Scalable Alkaline Hydrogen Production via Bifunctional Electrocatalysis

Levna Chacko, Sofer Zdeněk

Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Czech Republic

In response to the pressing need for sustainable energy solutions due to dwindling fossil fuels and environmental concerns, researchers are actively exploring cost-effective methods for the production of hydrogen, a clean fuel with immense potential. This study addresses the critical barrier of expensive platinum-group catalysts in electrochemical water splitting by presenting a novel approach to crafting affordable electrocatalysts from readily available transition metals such as cobalt, chromium, and iron [1]. The research unveils a straightforward and efficient synthesis technique for these versatile  $(TM)_{1/3}TaS_2$ -based catalysts [2], demonstrating their ability to facilitate both hydrogen evolution and oxygen evolution reactions - essential for complete water splitting in alkaline media. Notably, the electrocatalyst exhibits exceptional performance in a two-electrode setup, achieving low cell voltage at high current densities. By integrating experimental findings with theoretical computations, the study offers valuable insights into the charge transport mechanisms and their interplay with catalytic activity in this novel compound. This work marks a significant advancement in the development of costeffective solutions for hydrogen production, paving the way for a more sustainable future.

- 1. Yang, J.; Mohmad, A.R.; Wang, Y.; Fullon, R.; Song, X.; Zhao, F.; Bozkurt, I.; Augustin, M.; Santos, E.J.G.; Shin, H. S.; et al. Ultrahigh-current-density niobium disulfide catalysts for hydrogen evolution. *Nat. Mater* **2019**, *18*, 1309–1314; doi:10.1038/s41563-019-0463-8.
- Buravets, V.; Hosek, F.; Lapcak, L.; Miliutina, E.; Sajdl, P.; Elashnikov, R.; Švorčík, V.; Lyutakov, O. Beyond the Platinum Era—Scalable Preparation and Electrochemical Activation of TaS2 Flakes. ACS Appl. Mater. Interfaces 2023, 15, 5679–5686; doi:10.1021/acsami.2c20261.

### 0.S.I.C.3

### The impact of impurities on unconventional annealing of nanostructured copper

Michael Kerber<sup>1</sup>, Przemysław Suchecki<sup>2</sup>, Krzystof Sielicki<sup>2</sup>, Malgorzata Lewandowska<sup>2</sup>, Daria Setman<sup>1</sup>, <u>Agnieszka Krawczynska<sup>2</sup></u> <sup>1</sup>Faculty of Physics, University of Vienna, Boltzmanngasse 5,1090 Vienna, Austria <sup>2</sup>Faculty of Materials Science and Engineering, Warsaw University of Technology, 02-507 Warsaw, Poland

Pure nanostructured metals obtained by high pressure torsion are characterized by low thermal stability. The presence of impurities can significantly improve their thermal stability as these elements make the movement of grain boundaries more difficult. One can assume that while applying unconventional annealing nanostructured metals pure and with impurities will behave differently.

In this study, high hydrostatic pressure annealing was applied as an unconventional annealing technique because, unlike other techniques, it makes it possible to gain control over the evolution of a material microstructure. That evolution is retarded, since the high hydrostatic pressure applied during annealing suppresses diffusion processes. The experiments were performed on Cu ETP (electrolytic tough pitch) and DHP (deoxidized, oxygen-free copper with a residual phosphorus content). Samples were deformed by high pressure torsion to obtain nanostructures. Afterward, samples were annealed at 270°C for 15 minutes at atmospheric pressure and under high hydrostatic pressure of 6 GPa. After deformation and annealing, the microstructures were examined using transmission and scanning electron microscopy. The application of high hydrostatic pressure during annealing significantly hindered the grain growth in both samples in comparison with conventional annealing. Moreover, while applying high hydrostatic pressure in the case of Cu-DHP the grain growth was more uniform and the average grain size was smaller than in the case of Cu-ETP where abnormal grain growth was observed. Therefore, the addition of impurities also plays an important role during annealing under high hydrostatic pressure. The application of high hydrostatic pressure during annealing also improves the thermal stability of nanostructured materials.

Acknowledgment: This work was supported by the Polish National Science Center project 2021/03/Y/ST5/00253 Weave-UNISONO.

### 0.S.I.D.1

# Regulation of surface properties and structural defects of graphitic carbon nitride via oxygen doping and plasma treatment

Jana Petrović<sup>1</sup>, Željko Radovanović<sup>1</sup>, Bratislav Obradović<sup>2</sup>, Đorđe Janaćković<sup>3</sup>, Rada Petrović<sup>3</sup>

<sup>1</sup>Innovation Center of the Faculty of Technology and Metallurgy, Ltd, Belgrade, Serbia <sup>2</sup>University of Belgrade, Faculty of Physics, Belgrade, Serbia <sup>3</sup>University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia

Graphitic carbon nitride (CN) is gaining attraction as a photocatalyst for Cr(VI) reduction, thanks to its stability in acidic environments, facile preparation, low precursor cost, and moderate band gap (~2.7 eV). Still, its performance is limited primarily by inefficient separation of photogenerated electrons and holes. Recent studies show that introducing defects into CN structure can enhance its photocatalytic and photoelectric properties. The Dielectric Barrier Discharge (DBD) plasma process is emerging as an effective method to create defects in the form of oxygen-containing functional groups, which can act as electron-withdrawing sites, reducing charge carrier recombination, and thus improving photocatalytic activity. Additionally, increasing oxygen content by doping can facilitate the incorporation of more oxygen-based functional groups, like carboxyl, carbonyl, and hydroxyl. In this work, oxalic acid was used to synthesize O-doped CN, while the DBD plasma was employed to further modify the CN-based samples.

The properties of the photocatalysts were studied by XRD, FTIR, FESEM, EDS, PL, and DRS analysis, as well as by determination of the number of acidic surface functional groups. Photocatalytic reduction of Cr(VI) was tested at pH 3, under the simulated visible irradiation. It was shown that the primary framework of CN did not change during both doping and plasma treatment, while the content of acidic groups was significantly increased, and the recombination and band gap was decreased, but the photocatalytic efficiency was not improved significantly.

**Acknowledgement:** The authors wish to acknowledge the financial support for this research from The Ministry of Science, Technological Development and Innovation of the Republic of Serbia through project contracts No. 451-03-65/2024-03/200135 and 451-03-66/2024-03/200287.

### O.S.I.E.1

# Perfusion-based 3D *in vitro* cell culture model for osteosarcoma cells: Biological and chemical engineering perspectives

Ivana Banićević<sup>1</sup>, Mia Milošević<sup>1,2</sup>, Jelena Petrović<sup>1,2</sup>, Milena Milivojević<sup>3</sup>, Radmila Janković<sup>4</sup>, Jasmina Stojkovska<sup>1</sup>, Bojana Obradović<sup>1</sup> <sup>1</sup>University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia <sup>2</sup> Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia <sup>3</sup>University of Belgrade, Institute of Molecular Genetics and Genetic Engineering, Belgrade, Serbia <sup>4</sup>University of Belgrade, Faculty of Medicine, Belgrade, Serbia

Osteosarcoma is a primary malignant bone tumor affecting 3-4 per million people worldwide each year. The scarcity of novel therapies for osteosarcoma patients indicates persistent weaknesses in anticancer drug research, primarily due to heavy reliance on inadequate conventional models - cell monolayers and animals. 3D in vitro cell culture models, as physiologically more relevant have the potential to address this issue. Therefore, we aimed to develop a 3D in vitro osteosarcoma cell culture model based on bone-mimicking scaffolds and a perfusion bioreactor to achieve a closer imitation of the osteosarcoma cell microenvironment. Macroporous alginate hydrogel scaffolds with embedded hydroxyapatite particles (2 wt%) alginate, 2 wt% hydroxyapatite) were seeded with murine osteosarcoma cells (K7M2-wt) at the density 15x10<sup>6</sup> cells/cm<sup>3</sup> of scaffold volume. Cells were then cultivated in a perfusion biomimetic bioreactor ("3D Perfuse", Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia) for 7 days under continuous medium flow with a superficial velocity of 40 µm/s while static cell cultures served as control. In both perfusion and static cultures cells self-aggregated into spheroid-like structures, with those under perfusion conditions being more compact and larger. In addition, cells under perfusion exhibited higher metabolic activity, secreted more extracellular matrix, and possessed higher quantities of intracellular protein tubulin. Finally, a chemical engineering approach was employed to correlate cell biological characteristics with parameters in their microenvironment such as mass transport rates of oxygen and nutrients, and the presence of shear stresses in perfusion cultures. Mass transport of oxygen was modeled in both static and perfusion cultures and values of shear stresses in perfusion cultures were calculated as up to 2 mPa acting on the average spheroid. Overall, more favorable conditions were observed to be achieved in perfusion cultures, as further clarified by the chemical engineering approach.

O.S.I.E.2

### Size Matters: Exploring MXene-Cell Interactions

<u>Kateryna Diedkova</u><sup>1,2</sup>, Ena Enia<sup>1</sup>, Lita Grine<sup>1</sup>, Volodymyr Deineka<sup>1,2</sup>, Mārtiņš Borodušķis<sup>1</sup>, Ivan Baginskiy<sup>1,3</sup>, Oksana Petrichenko<sup>2</sup>, Veronika Zahorodna<sup>3</sup>, Oleksiy Gogotsi<sup>1,3</sup>, Maksym Pogorielov<sup>1,2</sup> <sup>1</sup>Sumy State University, Sumy, Ukraine <sup>2</sup>University of Latvia, Riga, Latvia <sup>3</sup>Materials Research Center LTD, Kyiv, Ukraine

A new type of two-dimensional layered nano-structure material, the MXenes, appeared on the research scene 13 years ago and, in turn, aroused keen interest in the biomedical domains of tissue engineering, biosensors, biological imaging, and tumor diagnosis. The large surface area, excellent conductivity, hydrophilicity, biocompatibility, biodegradability, and antibacterial activity are just some of the many distinctive qualities of MXene that set them apart from other nanomaterials. Nanomaterials can translocate biological barriers, distribute to different tissues, and, depending on their size and location, elicit different toxic effects on organisms [1]. The question of how different-sized MXene's nanolaminates interact with biological systems is becoming more and more important as a result of the new nanomaterial's extensive application in biomedical advancements. The aim of our research was to evaluate biocompatibility of  $Ti_3C_2$ ,  $Nb_2C$ ,  $V_2C$  MXenes with different lateral size.

 $Ti_3C_2$  MXenes with lateral size 300, 600, 1200 nm as suspension in DI and Nb<sub>2</sub>C with 600, 1200 nm, V<sub>2</sub>C with 300 and 600 nm in isopropanol were synthesized by Materials Research Center (Kyiv, Ukraine). The Zeta-sizer Nano ZS system was used to measure Z-potential and MXenes size. The cytotoxicity and proliferation effects of material size, concentration, and incubation time were evaluated using human keratinocytes (HaCaT) and human melanoma cell line (MaMel86a).

The findings regarding the cytotoxicity of various MXene types on keratinocytes and human melanoma cells revealed a dependence on the concentration, duration of incubation, and size of two-dimensional nanolaminates. Our results highlight how crucial it is to regulate the parameters of nanomaterials prior to biomedical application in order to prevent any negative effects and complications.

*Acknowledgments*: This research was funded by FP-21711-ZF-N-109 - Tailored Molecular Transport in Low-Dimensional Hybrid Materials from 1D Nanocrystals and 2D Nanosheets.

### **Reference:**

 Wang, X.; Cui, X.; Zhao, Y.; Chen, C. Nano-bio interactions: the implication of size-dependent biological effects of nanomaterials. *Sci. China Life Sci.* 2020, *63*, 1168–1182; doi:10.1007/s11427-020-1725-0

### O.S.I.E.3

# Thermodynamic characteristics of intermolecular interactions in the model bacterial membranes exposed to the LL-37 peptide action

<u>Katarzyna Pastuszak</u><sup>1</sup>, Małgorzata Jurak<sup>1</sup>, Marta Palusińska-Szysz<sup>2</sup> <sup>1</sup>Department of Interfacial Phenomena, Institute of Chemical Sciences, Faculty of Chemistry, Maria Curie-Skłodowska University, Maria Curie-Skłodowska Sq. 3, 20-031 Lublin, Poland <sup>2</sup>Department of Genetics and Microbiology, Institute of Biological Sciences, Faculty of Biology and Biotechnology, Maria Curie-Skłodowska University, Akademicka 19, 20-033 Lublin, Poland

LL-37, also referred to as human cathelicidin, is an antimicrobial peptide, naturally occurring in human organisms. The antibacterial activity results from the LL-37 molecule structure, which allows it to interact with phospholipids (PL) building the bacterial membranes. This can alter the PL molecules organization disrupting the continuity or permeability of the outer layer, consequently leading to the bacterial cell death. One of the species of bacteria against which the LL-37 could potentially be used is *Legionella gormanii*. *Legionella* spp. comprise four classes of phospholipids – phosphatidylcholine (PC), phosphatidylethanolamine (PE), phosphatidylglycerol (PG) and cardiolipin (CL). The composition of phospholipids in the membrane directly affects the physicochemical properties of the cell outer layer and influences the LL-37 peptide's membrane activity. The mutual proportions and content of each class can be modified by e.g. exogenous choline presence. The aim of these studies was to conduct the thermodynamic analysis of interactions occurring in model L. gormanii membranes with different phospholipid compositions, in the absence or presence of the LL-37 peptide. Phospholipids were isolated from L. gormanii bacteria cultured on a medium with (+choline) or without the addition of exogenous choline (-choline) and separated into four classes by means of thin-layer chromatography. The Langmuir monolayer technique was employed to prepare the model membranes of PL mixtures and individual classes with or without the LL-37 peptide in the subphase at 20 and 37 °C. This allowed obtaining the dependencies of surface pressure on the mean molecular area ( $\pi$ -A isotherms). Based on these experimental data, the excess area ( $A_e$ ), the excess Gibbs energy ( $\Delta G_e$ ) and the total Gibbs energy of mixing ( $\Delta G_m$ ) were determined. The obtained results revealed that PL-choline is characterized by stronger repulsive interactions between phospholipid molecules, wherein for PL+choline greater attraction occurs. Moreover, as indicated by  $A_e$  and  $\Delta G_e$  values, in the presence of LL-37, stronger repulsion or weakened attraction between PLs takes place, confirming the peptide's membrane-disturbing activity.

### 0.S.I.E.4

# Alginate microfibers with incorporated hydroxyapatite particles for 3D osteosarcoma cell cultures and rapid anticancer drug screening

Jelena Petrović<sup>1,2</sup>, Luka Bojić<sup>3</sup>, Milena Milivojević<sup>3</sup>, Ivana Banićević<sup>1</sup>, Radmila Janković<sup>4</sup>, Bojana Obradović<sup>1</sup>, Jasmina Stojkovska<sup>1</sup>

<sup>1</sup>University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia <sup>2</sup>Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia <sup>3</sup>University of Belgrade, Institute of Molecular Genetics and Genetic Engineering, Belgrade, Serbia <sup>4</sup>University of Belgrade, Faculty of Medicine, Belgrade, Serbia

Osteosarcoma is the most common primary malignant bone tumor and requires effective preclinical models to facilitate the development of new anticancer drugs. Current models include two-dimensional (2D) cell cultures and animal models, which cannot often fully replicate human cancer biology, leading to discrepancies in drug efficacy results between preclinical studies and clinical trials. This work aimed to develop a 3D osteosarcoma model based on alginate hydrogel with incorporated hydroxyapatite (HAP) particles, to create a simplified, yet reliable system for rapid anticancer drug screening.

Osteosarcoma cells (murine cell line K7M2-wt) were suspended ( $4 \times 10^{6}$  cells cm<sup>-3</sup>) in 2 wt. % alginate solution with or without 2 wt. % commercial HAP powder. The suspensions were manually extruded through a 26-gauge needle into a 0.18 M Ca<sup>2+</sup> gelling solution. The obtained microfibers were washed and cultured for up to 21 days. For anticancer drug testing, 3 cm of microfibers per well in a 96-well plate were treated with 0.25-20 µM doxorubicin solutions, while treated cells in monolayers served as controls. Histology (H&E staining) was used for the analysis of cell morphology and distribution, while the cell metabolic activity and the half-maximal inhibitory concentration ( $IC_{50}$ ) were determined by the MTT assay.

The 3D cultivation of osteosarcoma cells in alginate microfibers with and without HAP has shown that the microfibers supported cell viability, metabolic activity, and formation of cellular aggregates. The results of anticancer drug testing indicated higher resistance of the 3D cultures to doxorubicin compared to that in 2D: the IC<sub>50</sub> value for both 3D cultures of K7M2-wt cells was ~3  $\mu$ M, while that for the 2D culture was ~0.5  $\mu$ M. These results are consistent with the higher resistance to anticancer drugs observed in clinics compared to existing preclinical models and indicate the importance of developing more reliable *in vitro* models to improve preclinical platforms for drug discovery.

### O.S.II.A.1

#### Oxygen plasma-induced dry production of micro nanofibrillated cellulose (MNFC)

Patrick Gane<sup>1,2</sup>, Katarina Dimić-Mišić<sup>1</sup>, Monireh Imani<sup>1</sup>, Bratislav Obradović<sup>3</sup>, Milorad Kuraica<sup>3</sup>, Huy Quang Lê<sup>1</sup>, Matea Korica<sup>4</sup>, Mirjana Kostić<sup>2</sup>

<sup>1</sup>Aalto University, Department of Bioproducts and Biosystems, School of Chemical Engineering, 00076 Aalto, Helsinki, Finland

 <sup>2</sup>University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11000 Belgrade, Serbia
 <sup>3</sup>Faculty of Physics, University of Belgrade, Studentski trg 12, Belgrade 11001, Serbia
 <sup>4</sup>Innovation Center of Faculty of Technology and Metallurgy Ltd., University of Belgrade, Karnegijeva 4, Belgrade 11000, Serbia

Cellulose is set to become a major raw material which can enable the development of new sustainably resourced biodegradable composites supporting circular economy. Almost limitless possibilities exist for functionalising via the highly reactive hydroxyl groups, leading to the generation of tailored compatibility with a wide variety of industrial applications. Nanofibrillar cellulose comprising materials are some of the most promising lignocellulose derivatives from plant cellulose. Currently, their production capacity and economy are hindered by high chemical and energy consumption, the latter primarily during mechanical fibrillation of native fibre in aqueous suspension, and the negative limitation of very low solids content associated with the gel-like properties of the resulting final product. Eliminating the need for liquid water during fibrillation could, therefore, be transformative in respect to production feasibility, endproduct transportation and application. The application of oxygen gas dielectric barrier discharge (DBD) plasma on dry cellulose fibre is considered novel in respect to achieving onward nanofibrillation. The process is illustrated using once dried fibre coming from paper pulp manufacture, but in principle is not limited to wood source. The action of the oxygen plasma is to etch the liquid-water-free microcellulose fibre structure, simultaneously oxidising the glue-functioning hemicellulose, rendering it in turn potentially soluble. The absence of liquid water during this precursor process can deliver significant reduction in cost and environmental load. In addition, transport of plasma treated dry product to the point of application can decrease fuel consumption drastically and so bring yet further environmental benefits. This dry precursor process finally allows the nanopolymer crystalline-based cellulose fibrils to be readily released at the surface of the host refined microfibre. This can be undertaken subsequently, for example, using ultrasonication in aqueous medium, to form a micro nanofibrillated cellulose structure (MNFC), which generates the typical gellant effect in suspension, but newly without limitation of desired higher solids content.

### 0.S.II.A.2

# Enhancing selective deoxydehydration of biobased compounds for biobased nylon precursors using metal-doped solid rhenium catalysts

<u>Brigita Hočevar</u>, Maja Gabrič, Rok Pogorevc, Žan Lavrič, Matej Huš, Miha Grilc, Blaž Likozar Department of Catalysis and Chemical Reaction Engineering, National Institute of Chemistry, Liubljana, Slovenia

This study explores the catalytic potential of rhenium-based catalysts in deoxydehydration (DODH), specifically for the conversion of biomass-derived mucic acid into renewable adipates, crucial for nylon production. Our investigation involves various supported Re catalysts doped with different metals and considers the impact of catalyst pre-treatment conditions.

Re/C emerges as a highly effective DODH catalyst, with reductive pre-treatment playing a pivotal role, resulting in yields of up to 65 % for dehydroxylated products. DODH activity is intricately linked to the coexistence of metallic and high-valent Re sites, supported by thorough catalyst characterization. Sintering during thermal treatment is proposed to enhance bifunctional site formation, boosting overall catalytic performance.

We present a bifunctional reaction mechanism for DODH on monometallic Re catalysts, aligning with our experimental results and characterization findings. Additional doping with hydrogenation-capable metals significantly enhances the hydrogenation step toward the final adipic acid dimethyl ester. The synergistic combination of rhenium with metals like Pt or Pd notably improves conversion rates and selectivity toward the end product.

Our research highlights the potential of rhenium-based catalysts in sustainable adipate synthesis, emphasizing the importance of catalyst design and mechanistic understanding for advancing bio-based compound transformations in nylon precursor production.

In a nutshell, our research not only shows that rhenium catalysts can help make eco-friendly nylon but also gives us new insights into how to make these compounds in a more sustainable way. This is a step forward in creating environmentally friendly methods for producing materials like nylon.

#### 0.S.II.A.3

# Integration of functional oxides with silicon substrate for photo-electrochemical water splitting

Zoran Jovanović<sup>1,2</sup>, Urška Trstenjak<sup>2</sup>, Binbin Chen<sup>3</sup>, Darija Petković<sup>1</sup>, Gertjan Koster<sup>4</sup>, Matjaž Spreitzer<sup>2</sup>

<sup>1</sup>Laboratory of Physics, Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia

<sup>2</sup>Advanced Materials Department, Jozef Stefan Institute, Ljubljana, Slovenia <sup>3</sup>Key Laboratory of Polar Materials and Devices (MOE) and Department of Electronics, East China Normal University, 200241 Shanghai, China

<sup>4</sup>MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands

Epitaxial integration of oxides with semiconductor substrates is often limited by the lattice mismatch between the two material systems and their dissimilar chemical properties. As a consequence, the epitaxial growth of functional oxides on silicon requires atomically defined surfaces, which are most effectively prepared using SrO- or Sr-induced deoxidation and passivation. As-prepared surfaces enable overgrowth with various oxides for novel device applications. In most cases, the initial buffer layer is SrTiO<sub>3</sub> (STO), acting as a pseudo-substrate.

Noteworthy, the quality of the STO depends strongly on the method used and substrate pretreatment, which will be demonstrated on various templates. A case study, based on SrO-assisted deoxidation and controllable coverage of silicon surface with a layer(s) of spin-coated graphene oxide, will illustrate ability to grow a high-quality STO pseudo-substrate suitable for protection of silicon photoelectrode in the process of photo-electrochemical water splitting. The obtained results highlight the important quality of the overgrown STO film and underlying interface. The achieved integration of functional oxide with silicon provides robust route for solar-to-hydrogen energy conversion.

#### 0.S.II.A.4

### Synthesis and property of LaLuO<sub>3</sub>:Yb<sup>3+</sup> nanosize powders

<u>Oksana Korniienko</u>, Andrey Ragulya, Yuriy Yurchenko, Oleksandr Shyrokov, Tatiana Lobunets, Tamara Tomila, Marina Zamula, Valeriy Kolesnichenko Frantsevich Institute for Problem of Materials Science, NAS of Ukraine, Kyiv

The international scientific community has recently demonstrated a growing interest in materials with a perovskite structure. This is due to the potential for innovative applications of materials based on an ordered phase with a perovskite (ABO<sub>3</sub>) structure in a number of fields of science and technology. These include electrolytes for electrochemical devices such as solid oxide fuel cells (SOFCs), electrolyzers, sensors, hydrogen separation membranes and electrochemical catalytic reactors. The focus of this study is on materials based on an ordered structure, such as LaLuO<sub>3</sub> perovskite doped with Yb<sup>3+</sup> ions (1-5 mol.%). In the present work, a methodology for the synthesis of single-crystal nanopowder based on the above phase has been developed. A comprehensive study of the synthesized nanopowder was carried out using X-ray diffraction, microstructural, adsorption and structural methods, as well as infrared spectroscopy. The developed synthesis methodology enables the production of single-phase nanopowders, characterized by the formation of grains with a size of 30 to 90 nm (dependent on the selected mode of precursor heat treatment). The sintering of nanopowders was conducted via two methods: non-isothermal sintering in a dilatometer without pressure and spark plasma sintering at elevated pressure. The sintering process yielded ceramic samples with a density of approximately  $\sim$  97-99.5%. The results of the conducted research indicate that the maximum value of transparency of the LaLuO<sub>3</sub> sample doped with ytterbium (1 mol.%) is 63 to 69 % after sintering at a temperature of 1400 °C in the wavelength range of 6.8-7.8  $\mu$ m.

Acknowledgement: This work has been funded by project NATO G5769

#### **O.S.II.A.5**

### The influence of metal phase of novel Al<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub>/TiAl<sub>2</sub>O<sub>5</sub> composites obtained *via* slip casting method

Marcin Wachowski<sup>1</sup>, Justyna Zygmuntowicz<sup>2</sup>, Robert Kosturek<sup>1</sup>, Lucjan Śnieżek<sup>1</sup>, Paulina Piotrkiewicz<sup>2</sup>, Radosław Żurowski<sup>3</sup> <sup>1</sup>Faculty of Mechanical Engineering, Military University of Technology, 2 gen. S. Kaliskiego St., 00-908 Warsaw, Poland <sup>2</sup>Faculty of Materials Science and Engineering, Warsaw University of Technology, 141 Woloska St, 02-507 Warsaw, Poland <sup>3</sup>Faculty of Chemistry, Warsaw University of Technology, 3 Noakowskiego St, 00-664 Warsaw, Poland

This study aims to analyze the ceramic-metal composite  $Al_2O_3/TiO_2/TiAl_2O_5$  obtained using the slip-casting method. Samples containing 50 vol.% of the solid phase and 2 vol.% and 4 vol.% fractions of the metallic phase, were examined. Rheological investigations were performed. Measurements of shrinkage and density of the composites produced were determined. The phase composition of the obtained composite was investigated using SEM/EDS and the XRD techniques. Stereological analysis was performed as well. The slip-casting method enables the production of the proposed composite, reinforced by the presence of TiO<sub>2</sub> and TiAl<sub>2</sub>O<sub>5</sub>. With the increase in the content of the metallic phase in the composite, the thialite phase content increases but the relative density and volumetric shrinkage of the obtained composites decrease. Thialite grains are characterized by a size from 4 to 15  $\mu$ m, which leads to a low density of the samples. The results revealed that no significant effect of changing the metal phase content of the slurries used for fabricated composites was observed on the limiting grain growth of alumina during the sintering process of slip-casting composites.

#### O.S.II.B.4

### Alpha-pinene isomerization over TMAOH-treated multilayered Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene

<u>Bartosz Środa</u><sup>1</sup>, P. Miądlicki<sup>2</sup>, A. Wróblewska<sup>2</sup>, B. Zielińska<sup>1</sup> <sup>1</sup>Department of Nanomaterials Physicochemistry, Faculty of Chemical Technology and Engineering,

West Pomeranian University of Technology in Szczecin, Piastów Ave. 42, 71-065 Szczecin, Poland <sup>2</sup>Department of Catalytic and Sorbent Materials Engineering, Faculty of Chemical Technology and Engineering, West Pomeranian University of Technology in Szczecin, Piastów Ave. 42, 71-065 Szczecin, Poland

In the isomerization of  $\alpha$ -pinene, titanium dioxide (TiO<sub>2</sub>) is commonly used as a catalyst. One of the main reaction products of  $\alpha$ -pinene isomerization is camphene. Camphene is used in the food industry as a flavor additive. The main disadvantage of obtaining camphene by TiO<sub>2</sub> is its gradual deactivation with longer reaction times. As a result, scientists are actively searching for new catalysts that are stable, highly active, and capable of efficiently sustaining the reaction, as well as having shorter isomerization reaction times. This search has led to interest in MXenes, a broad family of two-dimensional materials. Within this family, titanium (IV) carbide (Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>) has attracted particular attention due to its unique properties and promising applications in organic heterogeneous catalysis. Nevertheless, MXenes are not without drawbacks. The main problem is the lack of a complete structure opening to increase the availability of active sites in heterogeneous catalysis [1].

Here, the effect of tetramethylammonium hydroxide (TMAOH) concentration on the delamination of multilayered  $Ti_3C_2T_x$  MXene was investigated. Multilayered  $Ti_3C_2T_x$  was synthesized by acid etching (48 % HF) of Al from MAX Phase. Next, the obtained  $Ti_3C_2T_x$  was dispersed in 0.2, 0.3, and 0.4 M TMAOH solutions, respectively. Firstly 100 mg of MXene was dispersed in 10 mL of TMAOH solution. The reaction was carried out for 12 hours. After that delaminated MXenes were washed via centrifugation. The pristine  $Ti_3C_2T_x$  and  $Ti_3C_2T_x$  treated with 0.2, 0.3, and 0.4 M TMAOH solutions were used as catalysts in the reaction of  $\alpha$ -pinene isomerization (160 °C, 6 h). Morphological studies showed that the multilayered MXene became thinner as the concentration of TMAOH increased. All studied samples were characterized using different techniques such as scanning electron microscopy (SEM), X-ray diffraction (XRD), Raman spectroscopy, thermogravimetric analysis (TGA), and X-ray spectroscopy (XPS).

*Acknowledgment:* This work was financially supported by the National Science Centre Poland (Preludium Bis 2, 2020/39/O/ST5/01340).

#### **References:**

1. E. Gastao,US Pat.US 2551795 A, Du Pont, 8 May 1951 <u>https://doi.org/10.1039/9781847552044-00024</u>.

#### O.S.II.B.5

### Insight into electrocatalytic oxygen evolution the reaction mechanism in the presence of Borophene/Ni<sup>2+</sup> with induced crystal lattice defects and porosity

Ewa Mijowska, Klaudia Zielinkiewicz, Grzegorz Leniec

West Pomeranian University of Technology, Szczecin Faculty of Chemical Technology and Engineering, Department of Nanomaterials Physicochemistry, Piastow Ave. 45, 70-311 Szczecin, Poland

Ir/Ru-based electrocatalysts have been extensively studied for the oxygen evolution reaction (OER). However, a sluggish anodic process requires a substantial overpotential to achieve a significant current. This inefficiency in water electrolysis results in low oxygen production rates. Therefore, the rational design and comprehensive characterization of promising electrocatalysts is crucial for the advancing of energy conversion technologies. Deep characterization under reaction conditions is necessary to uncover the chemical nature and activity descriptors of the OER mechanism, which, despite being ideally-studies, remains complex and enigmatic.

In this context, we present a novel approach to understanding the OER mechanism using a borophene-based catalyst supported by  $Ni(NO_3)_2$  (U-Borophene+ $Ni(NO_3)_2$ ) with induced lattice defects and porosity. The catalyst was synthesized via chemical intercalation, effectively exfoliating bulk boron into few-layered borophene. This material was then combined with  $Ni(NO_3)_2$ · $6H_2O$  and subjected to rapid dehydration, inducing crystal lattice defects and porosity. A series of ex-situ techniques, including nitrogen adsorption/desorption, XPS, EPR and XRD were employed to characterize the catalyst. Electrochemical experiments confirmed that the U-Borophene+ $Ni(NO_3)_2$  electrocatalyst possesses a tailored structure with active sites that facilitate both conventional OER and lattice oxygen ER. As a result, this catalyst demonstrates an overpotential of 169.56 mV at 10 mA/cm<sup>2</sup> and a low Tafel slope of 31 mV per decade in a 1 M potassium hydroxide electrolyte, outperforming ruthenium oxide and other leading electrocatalysts. Thus, this study not only advances the development of effective borophene-based OER catalysts by highlighting the crucial physicochemical features of efficient electrocatalysts but also contributes to a deeper understanding of the reaction mechanism.

#### **O.S.II.B.6**

# Exploring the potential of Na<sub>4</sub>Fe<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>P<sub>2</sub>O<sub>7</sub>/C as a cathode material for Na-ion rechargeable batteries

<u>Milica Vujković</u><sup>1,2</sup>, Aleksandra Gezović Miljanić<sup>3</sup>, Jana Mišurović<sup>3</sup>, Alen Vižintin<sup>4</sup>, Slavko Mentus<sup>1,5</sup> Robert Dominko<sup>4</sup> <sup>1</sup>University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia <sup>2</sup>Center for Interdisciplinary and Multidisciplinary Studies, University of Montenegro, Podgorica, Montenegro <sup>3</sup>Faculty of Metallurgy and Technology, University of Montenegro, Podgorica, Montenegro <sup>4</sup>National Institute of Chemistry, Ljubljana, Slovenia <sup>5</sup>Serbian Academy of Sciences and Arts, Belgrade, Serbia

While layered/spinel oxide and olivine phosphate cathodes, particularly Li(Co-Ni-Mn)O<sub>2</sub>, dominate the Li-ion battery market, Prussian blue analogs, NASICON-type and layered oxide structures are available in emerging Na-ion prototypes. In both cases, the development of affordable, safe, and sustainable cathode structures, that deliver high redox potential/specific capacity, remains a significant challenge. With economic & environmental aspects as a priority, we have dedicated all our efforts to developing Li, Co, and V-free polyanionic cathodes for Na-ion batteries, using abundant and eco-friendly elements such as sodium and iron.

In our previous studies [1,2], we addressed synthesis challenges of polyanionic cathode,  $Na_4Fe_3(PO_4)_2P_2O_7$  (NFPP), offering guidelines for its sol-gel route. The optimized composite reached theoretical capacity (129 mAh g<sup>-1</sup>) at 1C in 6M NaNO<sub>3</sub>. Herein, we will show its cyclic performance in a coin-cell configuration, using NaPF<sub>6</sub>/EC+DMC with and without additives. Unlike the capacity decline observed in an aqueous electrolyte, even in highly concentrated Na-based formulations, stable capacity was maintained in an organic electrolyte over 100 charge/discharge cycles. However, a somewhat lower capacity was registered (~93 mAh g<sup>-1</sup> at C/10 over 1.8 – 3.7 V range), especially at higher current rates. Sodiation/desodiation mechanism of NFPP in an organic electrolyte will be investigated. The talk will highlight the potential of NFPP as a novel cathode formulation for Na-ion batteries and further opportunities.

*Acknowledgments:* The research was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia - Contract No: 451-03-66/2024-03/200146 and Serbia-Germany Bilateral project No.9.

#### **References:**

- 1. A. Gezović, M. Vujković et al, Energy Storage Materials, 37, 2021, 243-273.
- 2. A. Gezović, et al, Electrochimica Acta, 476, 2024, 143718.

#### O.S.II.E.5

#### Laser-Induced Self-Organized Microrod Arrays For Osteoblasts Proliferation

<u>I. Gnilitskyi</u><sup>1,2,3</sup>, K. Diedkova<sup>4,5</sup>, Anton Roshchupkin<sup>4</sup>, Milena Yalyzhko<sup>4</sup>, M. Pogorielov<sup>4,5</sup>, A. V. Zayats<sup>1</sup>

<sup>1</sup>Department of Physics and London Centre for Nanotechnology, King's College London, Strand, London WC2R 2LS, UK

<sup>2</sup>Department of Applied Physics, Lviv Polytechnic National University, 79013 Lviv, Ukraine <sup>3</sup>"NoviNano Lab" LLC, 5 Pasternaka, Lviv, Ukraine

<sup>4</sup>Biomedical Research Center, Sumy State University, 31 Sanatorna St, Sumy 40007, Ukraine <sup>5</sup>University of Latvia, Institute of Atomic Physics and Spectroscopy, 3 Jelgavas St, Riga LV-1004, Latvia

Ultrafast laser pulses, with durations in the femtosecond range, have become an important technology in shaping and modifying materials, particularly for creating structures at the nanoscale. This technique offers several advantages over traditional lasers with longer pulses. Femtosecond lasers achieve material removal through non-thermal processes, which is ideal for situations where heat damage needs to be minimized, especially when working with delicate materials like dielectrics and semiconductors. Another benefit is the ability to directly create microscopic features under ambient conditions, eliminating the need for complex vacuum environments. In this paper we explore the formation of microrod assemblies on metal surfaces (specifically, a titanium alloy) through self-organization triggered by ultrashort laser pulses. This method allows rapid, direct formation of self-assembled microscopic structures across large areas. The microrods typically have a diameter ranging from 5 to 25 micrometers and a height between 5 and 30 micrometers. Their arrangement is quasi-periodic, with spacing between 5 and 20 micrometers. By adjusting the laser irradiation settings, the geometrical dimensions of the microrods can be controlled. The formation of these laser-induced structures occurs within the ablation zone and is a cumulative effect caused by repeated laser pulses. The self-organized microrod arrays hold significant potential for developing structured surfaces with applications in catalysis and biomedicine. To evaluate the application of such microstructured surfaces in biomedicine, we investigated their biocompatibility and ability to support cell proliferation. Given the prevalent use of titanium (Ti) alloys in orthopedics, we employed the MG63 cell line to assess surface biocompatibility towards osteogenic cells. The samples were sterilized by exposure to 70 % ethanol solutions for 1 hour, followed by three washes with sterile PBS. Cells were then seeded onto the samples at a density of 104 cells/well. with 2 mL of medium added to each well. The culture medium was refreshed every 2 days, and cell viability was evaluated at 1, 3, and 7 days using the resazurin reduction assay. At the final time point, the samples were stained with ActinRed 555 (cytoskeleton) and Hoechst 33342 (nuclei) to assess cell morphology and their distribution on the treated surfaces. The results indicate that the microstructured surfaces promote cell adhesion and proliferation, demonstrating a significantly higher proliferation rate compared to the untreated control surfaces. Fluorescent staining revealed uniform cell distribution across the surface, with higher confluency compared to polished surfaces. These findings suggest that the novel microstructured surfaces hold promise for biomedical applications, particularly in orthopedics and cardiovascular implants.

#### O.S.II.E.6

# Antibacterial effectiveness and safety of MXene-loaded electrospun polycaprolactone membranes for photothermal ablation

<u>Viktoriia Korniienko</u><sup>1,2</sup>, Keelan Warren<sup>1</sup>, Yuliia Varava<sup>2</sup>, Valeriia Korniienko<sup>2</sup>, Kateryna Diedkova<sup>1</sup>, Veronika Zahorodna<sup>3</sup>, Oleksiy Gogotsi<sup>3</sup>, Una Riekstina<sup>1</sup>, Maksym Pogorielov<sup>1,2</sup>

<sup>1</sup>University of Latvia, Riga, Latvia <sup>2</sup>Sumy State University, Sumy, Ukraine, <sup>3</sup>CARBON-UKRAINE Ltd., Kiev, Ukraine

Recent advancements in biomedical materials have introduced alternatives for treating bacterial infections without antibiotics. Photothermal therapy (PTT) utilizes photothermal agents like MXene to convert light absorption into heat, effectively eliminating bacteria. This study investigates the optimal parameters of laser exposure for effective antibacterial photothermal therapy using MXene-loaded electrospun polycaprolactone (PCL) membrane.

Before the MXene immobilization, the as-spun PCL membranes were treated with oxygen plasma, improving the surface hydrophilicity. The Ti<sub>3</sub>C<sub>2</sub> MXene solution with PCL membranes was sonicated and left for 3 h to immobilize MXene on the PCL membranes. The antibacterial potential of PTT (laser regimens - 3 watts/10 Hz for 5 min and 4 watts/50 Hz for 10 min) were assessed against *Escherichia coli* (*E. coli*, ATCC 25922) using colony forming unit method (CFU) and resazurin reduction assay. Cytotoxicity and biocompatibility of Mxene-loaded membrane and safety of laser regimens were evaluated on human dermal fibroblasts (D6) using resazurin reduction assay and fluorescent microscopy.

MXene-loaded PCL membrane demonstrated appropriate cell adhesion and proliferation with uniform fibroblast distribution after laser exposure. Results of PTT experiment demonstrated negligible effects on bacterial viability after 24 hours of laser irradiation. MXene-loaded membranes exhibited highly effective bacteria-killing efficiencies (99.9 % against *E. coli*) under 4 watts/50 Hz laser parameters for 10 min.

These findings highlight MXene's potential for antibacterial treatment without cytotoxic effects on human skin cells, emphasizing its role in combating bacterial infections. However, for this potential to be fully harnessed, further studies are crucial to establish a clear protocol for antibacterial PTT. This includes considerations such as the type of irradiation mode, intensity, and exposure time.

**Acknowledgment:** This research received support from FP-21711-ZF-N-109 - Tailored Molecular Transport in Low-Dimensional Hybrid Materials from 1D Nanocrystals and 2D Nanosheets.

#### O.S.II.E.7

# *In vitro* electrophoresis to uncover mechanism of fragmentation of DNA by MXene in DNA comet assay

Inna Chorna<sup>1</sup>, Zhanna Klishchova<sup>1,2</sup>, Artem Shmatkov<sup>1</sup>, Anton Roshchupkin<sup>1</sup>, Illya Yanko<sup>1</sup>, Sergiy Dukhnovskiy<sup>3</sup>, Ivan Baginskiy<sup>3</sup>, Veronika Zahorodna<sup>3</sup>, Iryna Roslyk<sup>3</sup>, Oleksiy Gogotsi<sup>3</sup>, Maksym Pogorielov<sup>1,4</sup>, <u>Sergiy Kyrylenko<sup>1</sup></u> <sup>1</sup>Sumy State University, Sumy, Ukraine <sup>2</sup>Federal University of Lavras UFLA, Lavras, Brazil <sup>3</sup>Materials Research Centre LTD, Kyiv, Ukraine <sup>4</sup>University of Latvia, Riga, Latvia

MXenes is a new family of 2D materials with promising potential in various applications due to their unique properties and structure. It is evident that MXenes will soon be used in many applications in close contact with the human body. Moreover, MXenes are intensively explored in various biomedical applications, including cancer treatment, hemodialysis, neural guidance conduits, biosensors etc. Studies have shown minimal toxicity, good biocompatibility and favorable interactions with biological systems of MXenes, paving the way for their use in biomedicine. Nevertheless, genotoxicity of MXenes has not been yet addressed. We have previously shown by DNA comet assay that both  $Ti_3C_2$  and  $Nb_4C_3$  MXenes induce robust appearance of DNA comets in various cells in cultures. The nature of the observed DNA fragmentation however remains obscure. Thus, we could not verify fragmentation of the DNA by alternative methods. We hypothesized that the sharp edges of MXenes can cause DNA breaks when they move in electric field under conditions of gel electrophoresis. To verify this hypothesis, we developed the technique of in-vitro electrophoresis. For this, we cultured the cells in 6-well plates and loaded them with MXenes. Then, using 3D printed polymer inserts, we placed into the cell culture wells two platinum electrodes at the opposite sides of the wells and applied electric field, similar to conditions of the DNA comet assay. We expected that the MXene loaded cells would develop apoptosis or necrosis when subjected to the electric field. The conditions of electrophoresis indeed impaired viability of the cells, most probably due to changes in pH. However, we could not reliably detect the increased level of cell death in cells with MXenes under conditions of electrophoresis. The results of the in-vitro electrophoresis and the nature of DNA comets remain a subject of debates.

Acknowledgments: Supported by the Air Force Office of Scientific Research via EOARD project P809, HORIZON-MSCA-2022-SE-01-01 project #101131147 ESCULAPE, LRC grant #2023/1-0243, grant #3050 of the EURIZON H2020 project 871072, CAPES project #23038.003877/2022-44 SOLIDARIEDADE ACADÊMICA, project #0124U000637 of the Ministry of Education and Science of Ukraine, ERASMUS-JMO-2022-CHAIR project #101085451 CircuMed, ERASMUS-JMO-2023-MODULE project #101127618 MedFood.

### Advanced composite nanomaterials fabricated by high-pressure torsion technique

Piotr Bazarnik<sup>1</sup>, Yi Huang<sup>2</sup>, Małgorzata Lewandowska<sup>1</sup>, Terence G. Langdon<sup>2</sup> <sup>1</sup>Warsaw University of Technology, Faculty of Materials Science, Woloska 141, 02-507, Poland <sup>2</sup>Materials Research Group, Department of Mechanical Engineering, University of Southampton, Southampton SO17 1BJ, UK

Nanostructured alloys have attracted significant interest due to their unique sets of properties which are not achievable in coarse-grained polycrystalline materials. In recent years, a new approach for the formation of hybrid multi-layer materials by joining dissimilar materials was introduced. Due to the fact that this is a new approach, to date there are only limited numbers of demonstrations of any alternative methods of fabricating high-performance material by bonding dissimilar bulk metals to form new metal systems through High-Pressure Torsion (HPT).

This work describes the use of HPT to produce various nanostructured composites from Cu and AI based systems reinforced with various metallic and ceramic phases. All systems were fabricated by HPT under 6.0 GPa of compression pressure and under various numbers of turns. The samples were examined by X-ray diffraction, scanning and transmission electron microscopy (SEM-TEM), energy dispersive spectrometry (EDX), microhardness measurements and tensile tests. A microstructural study after HPT processing showed formation of vortices like structures and particle agglomerates which were further fragmented and distributed uniformly over the matrix through increases in the numbers of HPT turns. In some cases, a solid-state diffusion between the elements was observed. Mechanical properties of such composites were 200-600% higher than those reported for initial materials. The results demonstrate that HPT offers a significant opportunity for producing novel nanostructured multilayered composites with unique mechanical properties.

### Aqueous dispersions of basic copper salts. Electric double layer and ion exchange

Marek Kosmulski Lublin University of Technology, Poland

Basic copper chlorides and sulfates are common minerals, and they occur as products of corrosion of copper and of its alloys. They are sparingly soluble in water, although their solubility is higher than that of Cu(OH)<sub>2</sub>. They are widely applied in horticulture as fungicides and as a source of copper for feeding livestock. Basic copper chlorides and sulfates were found in historical pieces of art. The other basic copper salts are less well-known. The pH-neutral dispersions of basic copper salts are stable against coagulation, but they are chemically stable over a narrow pH range. They dissolve in acids and they convert into CuO at pH>10.

The electrokinetic properties of various basic copper salts are similar, that is, they are rather insensitive to the nature of the anion. Basic copper salts show the isoelectric point IEP at pH about 9, which matches the IEP of CuO reported in the literature [1]. This result is against expectations, because anions like sulfate and chloride are less basic than hydroxide anion, thus lower IEP in basic salts than in corresponding oxides or hydroxides is expected. A surprisingly high IEP of basic copper salts suggests that a thin surface layer of a basic salt is converted into CuO also at pH about 9, and the thin shell of the particles rather than their core is responsible for the surface charging.

Basic copper salts are anion-exchangers, for example, basic copper sulfate can be completely converted into basic copper chloride by immersion in NaCl solution, and also basic copper chloride can be completely converted into basic copper sulfate by immersion in  $Na_2SO_4$  solution.

#### **Reference:**

1. M. Kosmulski, Electrokinetic potential of precipitates obtained from CuSO4, alkali halides, and NaOH, Materials Chemistry and Physics 319: 129385 (2024).

# Distance dependence of MXene-induced fluorescence energy transfer and applications in single-molecule biosensing

<u>Carmen Lorena Manzanares-Palenzuela</u><sup>1,2</sup>, Dahnan Spurling<sup>3</sup>, Alan Szalai<sup>1,4</sup>, Ece Büber<sup>1</sup>, Tim Schröder<sup>1</sup>, Valeria Nicolosi<sup>3</sup>, Philip Tinnefeld<sup>1</sup>

<sup>1</sup>Department of Chemistry and Center for NanoScience, Ludwig-Maximilians-University, Butenandtstraße 5-13, 81377, Munich, Germany

<sup>2</sup>CNRS, Centrale Lille, University Polytechnique Hauts-de-France, UMR 520 - IEMN, LIA LICS, University of Lille, Lille, France

<sup>3</sup>School of Chemistry, Trinity College Dublin, Dublin 2, Ireland

<sup>4</sup>CONICET Centro de Investigaciones en Bionanociencias (CIBION), Polo Científico Tecnológico Godoy Cruz 2390, Buenos Aires, Argentina

MXenes, discovered in 2011, have been widely recognized as 2D materials with potential applications in energy storage, electromagnetic shielding, and optoelectronics [1]. The energy transfer properties of these materials are still not fully understood, and this knowledge may have implications in various fields.

In this study, we utilized single-molecule confocal fluorescence microscopy and DNA origami nanopositioners to explore the distance-dependent intensity and lifetime of an emitter [2] (ATTO 542) placed on transparent thin films of spin-coated Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene 2D flakes [3]. Each DNA origami structure was created to carry a single dye molecule at predetermined heights. We developed a specific immobilization chemistry for DNA origami nanostructures based on the interaction between glycine and MXene, which allowed us to precisely control their orientation on the surface.

Our research showed that when the dye was positioned between 1 nm and 8 nm from the surface, the fluorescence quenching followed a distance dependence of  $d^{-3}$ . These findings are consistent with the well-known Förster mechanism of near-field energy transfer with transparent conductors at the bulk level [4,5]. MXenes have the potential to serve as short-range spectroscopic nano-rulers for measuring biomolecular processes, providing a high level of sensitivity at a distance range that conventional energy transfer tools cannot reach. In this context, we demonstrate the utility of MXenes in single-molecule biosensing, focusing on model cell membranes as exemplary study systems. MXenes offer unique capabilities to uncover nanoscale dynamic processes that are intricately embedded in the ultrathin membrane architecture of cells.

#### **References:**

- 1. Gogotsi, Y.; Anisori, B. The rise of MXenes. ACS Nano 2019, 13, 8491.
- Isbaner. S.; Karedla, N.; Kaminska, I.; Ruhlandt, D.; Raab, M.; Bohlen, J.; Chizhik, A.; Gregor, I.; Tinnefeld, P.; Enderlein, J.; Tsukanov, R. Axial Colocalization of Single Molecules with Nanometer Accuracy Using Metal-Induced Energy Transfer. *Nano. Lett.* 2019, 19, 4257.
- 3. Zhang, C.J.; Anasori, B.; Seral-Ascaso, A.; Park, S.H.; McEvoy, N.; Shmeliov, A.; Duesberg, G.S.; Coleman, J.N.; Gogotsi, Y.; Nicolosi, V. Transparent, Flexible, and Conductive 2D Titanium Carbide (MXene) Films with High Volumetric Capacitance. *Adv. Mater.* **2017**, *29*, 1702678.
- 4. Moerland, R.; Hoogenboom, J. Subnanometer-accuracy optical distance ruler based on fluorescence quenching by transparent conductors. *Optica* **2016**, *3*, 112–117.
- Chance, R.R.; Miller, A.H.; Prock, A.; Silbey, R. Fluorescence and energy transfer near interfaces: The complete and quantitative description of the Eu+3/mirror systems. J. Chem. Phys. 1975, 63, 1589–1595.

### Integration of MXenes in Ceramic Matrices for Enhanced Material Properties

<u>Maxim Sokol</u>, Barak Ratzker, Or Messer Tel Aviv University, P.O.B 39040, Ramat Aviv 6997801, Israel

MXene materials have garnered significant attention for their versatility, sparking interest in their integration with metal or ceramic matrices to develop advanced nanocomposites. This study introduces a straightforward method for producing bulk MXene/ceramic nanocomposites via the blending of MXene with ceramic particles, followed by field-assisted sintering. Using the Ti<sub>3</sub>C<sub>2</sub>T<sub>z</sub>/alumina system as a model, we explored the impact of MXene integration on the densification behavior and properties of the nanocomposites. Our findings reveal that MXene notably accelerates the densification process at lower temperatures and ensures a uniform distribution of  $Ti_3C_2T_z$  MXene along the alumina grain boundaries. The resultant Ti<sub>3</sub>C<sub>2</sub>T<sub>z</sub>/alumina nanocomposites demonstrate enhanced electrical conductivity and strong light absorption capabilities, although there is a reduction in hardness attributed to the weakening of grain boundaries by the intergranular layered MXene. Further, utilizing multilayered  $Ti_3C_2T_2$ as a precursor enables the formation of composites with a plate-like TiCx morphology. We propose that the techniques described here are extendable to metals and other common ceramics, with the potential for tailoring MXene type, size, composition, and termination groups to align with various oxides, nitrides, or carbides based on targeted properties. This study outlines a strategic framework for leveraging MXene's diversity and adaptability in crafting tunable advanced nanocomposites.

### Utilizing Interferometric Scattering Microscopy to Explore Ion Dynamics within Single Two-Dimensional MXene Nanoparticles

<u>Mohsen Beladi Mousavi</u><sup>1</sup>, Franz Gröbmeyer<sup>1</sup>, Christoph Gruber<sup>1</sup>, Kyle Matthews<sup>2</sup>, Kateryna Shevchuk<sup>2</sup>, Alex Inman<sup>2</sup>, John Wang<sup>2</sup>, Yury Gogotsi<sup>2</sup>, Emiliano Cortes<sup>1</sup> <sup>1</sup>Ludwig-Maximilians-Universität (LMU) Munich, Faculty of physics, Königinstraße 10, 80539 Munich, Germany

<sup>2</sup>A.J. Drexel Nanomaterials Institute and Department of Materials Science and Engineering, Drexel University, 3141 Chestnut Street, Philadelphia, PA, 19104, United States

MXene, a novel class of two-dimensional materials, holds significant potential in revolutionizing energy storage systems due to its exceptional electrical conductivity. large surface area, and ability to accommodate various ions, enhancing the performance of batteries and supercapacitors.<sup>[1-2]</sup> In this pioneering study, state-of-the-art operando microscopy, *i.e.*, interferometric scattering microscopy (iSCAT) reveals the intricacies of ion diffusion within MXene nanostructures at the scale of individual nanoparticles. The research delivers an indepth analysis of the dynamics of ion transport and charge transfer, shaped by variables such as ion size, hydrophilicity, and the nature of the solvent used. The deployment of non-invasive operando microscopy for live tracking has shed light on the influence of these variables on ion mobility within MXene frameworks. Notably, the research has identified how ion diffusion contributes to power density at the nanoparticle level, thus enhancing our ability to precisely measure the boundaries of charge transport in MXene films. These breakthroughs are vital for the advancement of energy storage technologies, providing a clearer understanding of ion movement at the nanoscale and its implications for the efficacy of high-performance materials. This investigation lays the groundwork for future enhancements in energy storage devices, suggesting that fine-tuning ion transport could markedly elevate power density and efficiency.

#### **References:**

- 1. Vahid Mohammadi, A.; Rosen, J.; Gogotsi, Y. The world of two-dimensional carbides and nitrides (MXenes). *Science* **2021**, *372*, eabf1581.
- 2. Li, X.; Huang, Z.; Shuck, C.E.; Liang, G.; Gogotsi, Y.; Zhi, C. MXene chemistry, electrochemistry and energy storage applications. *Nat. Rev. Chem.* **2022**, *6*, 389–404.

#### O.S.III.D.2

#### Photocatalytic coatings with Ce-loaded zeolites

Kristina Mojsilović<sup>1</sup>, Srna Stojanović<sup>2</sup>, Maria Serdechnova<sup>3</sup>, Carsten Blawert<sup>3</sup>, Ljiljana Damjanović-Vasilić<sup>2</sup>, Mikhail L. Zheludkevich<sup>3,4</sup>, Stevan Stojadinović<sup>1</sup>, <u>Rastko Vasilić<sup>1</sup></u>
 <sup>1</sup>University of Belgrade, Faculty of Physics, Studentski trg 12-16, 11000 Belgrade, Serbia
 <sup>2</sup>University of Belgrade, Faculty of Physical Chemistry, Studentski trg 12-16, 11000 Belgrade, Serbia
 <sup>3</sup>Institute of Surface Science, Helmholtz-Zentrum Hereon, Max-Planck-Straße 1, 21502 Geesthacht, Germany
 <sup>4</sup>Institute of Materials Science, Faculty of Engineering, Kiel University, Kaiserstraße 2, 24143 Kiel, Germany

Common photocatalytic processes are carried out in reactors where photocatalysts are in the form of powders (particles), resulting in drawbacks such as agglomeration, obstruction of light penetration, necessity of separation from the reaction medium, and so on. To avoid these obstacles, the formation of immobilized composite photocatalysts by plasma electrolytic oxidation (PEO) proved itself as a valuable tool for producing cost- and time-effective photocatalysts. Furthermore, PEO processing enables the incorporation of electrolyte components (including particles) into coatings, providing the pathway for tailoring the properties of such composite coatings. An innovative immobilization of Ce-loaded synthetic (13X and ZSM-5) and natural (clinoptilolite) zeolites on an inexpensive support using PEO processing proved to be beneficial when both photocatalytic and corrosion protection properties are of interest.

All prepared coatings contain elements originating from the substrate and from the electrolyte. Cerium concentration is very low for all coatings with incorporated Ce-loaded zeolites. Generally, coatings with incorporated Ce-loaded zeolites show higher photoactivity then those with pure zeolites. The highest photocatalytic activity is observed for coating with immobilized Ce-loaded 13X zeolite. The effect of Ce is not too strongly pronounced on anti-corrosion properties of coatings with incorporated Ce-loaded zeolites due to its low concentration but it is still detectable.

#### **O.S.III.D.3**

#### Effect of plasma treatment on surface chemistry and morphology of jute fibers

<u>Mirjana Kostić</u><sup>1</sup>, Marija Milošević<sup>1</sup>, Bratislav Obradović<sup>2</sup>, Matea Korica<sup>3</sup>, Alenka Vesel<sup>4</sup>, Aleksandra Ivanovska<sup>3</sup>, Milorad Kuraica<sup>2</sup>, Zorica Svirčev<sup>5,6</sup> <sup>1</sup>Faculty of Technology and Metallurgy, University of Belgrade, Serbia <sup>2</sup>Faculty of Physics, University of Belgrade, Serbia <sup>3</sup>Innovation Center of the Faculty of Technology and Metallurgy, University of Belgrade, Serbia <sup>4</sup>Jožef Stefan Institute, Ljubljana, Slovenia <sup>5</sup>Faculty of Sciences, University of Novi Sad, Serbia <sup>6</sup>Faculty of Science and Engineering, Åbo Akademi University, Finland

In this work, jute fibers, in the form of fabrics, were subjected to atmospheric pressure dielectric barrier discharge (DBD) under different conditions (150 Hz or 300 Hz, air as working gas, constant time of 120 s) to tailor their surface chemistry and morphology and consequently properties. The effect of DBD treatment on the surface chemistry of jute fibers was investigated by ATR-FTIR, XPS, and electrokinetic measurements, while FE-SEM and AFM were used to assess the changes in the surface morphology of treated fibers. The electrokinetic measurements and sorption properties monitored by wetting time and capillary height measurements were used to follow aging processes in DBD-treated jute fibers. Changes in the jute fiber surface chemistry, such as more exposed cellulose on the fiber surface due to the removal of surface impurities and non-cellulosic components, decreased lignin and hemicellulose contents, in parallel with cellulose oxidation, and morphology (about 3.2 times higher average roughness, i.e., formation of new pores and capillaries as a result of the intensive etching and ablation of the fiber surface layers) were more pronounced in the case of lower frequency DBD treatment. The obtained results also revealed that both DBD treatments improved the wettability of jute fibers, with lower frequency DBD treatment being more efficient. This investigation confirmed the significant influence of aging effects in jute fibers' functionalization using plasma.

*Acknowledgment*: This research was funded by the Science Fund of the Republic of Serbia (#7726976), Integrated Strategy for Rehabilitation of Disturbed Land Surfaces and Control of Air Pollution - RECAP.

#### O.S.III.D.4

#### Performance Properties of Concrete Produced Using Recycled Polymer Shot

<u>Marcin Małek</u><sup>1</sup>, Katarzyna Jasik<sup>2</sup>, Emil Kardaszuk<sup>1</sup>, Michał Gregorczyk<sup>1</sup>, Waldemar Łasica<sup>1</sup>, Janusz Kluczyński<sup>2</sup>

<sup>1</sup>Military University of Technology, Faculty of Civil Engineering and Geodesy, Testing Laboratory, Gen. S. Kaliskiego 2, 00-908 Warsaw, Poland

<sup>2</sup>Military University of Technology, Faculty of Mechanical Engineering, Institute of Robots & Machine Design, Gen. S. Kaliskiego 2, 00-908 Warsaw, Poland

In recent years, the production of plastics has increased dynamically, leading to a significant rise in waste generation. These wastes pose significant environmental and health problems. Three main waste disposal methods are commonly employed: incineration, landfilling, and recycling. Among these methods, recycling is considered the best disposal method due to its environmental and economic benefits. Effective recycling methods constitute a crucial area of research interest in various industrial sectors, especially in construction. Incorporating plastic waste into concrete not only minimizes the amount of disposed waste but also improves the final properties of concrete. This study aimed to evaluate the properties of concrete with the addition of polymer shot in amounts of 5 and 10 % of the final sample mass. Physical tests were conducted, including density measurement, thermal conductivity coefficient, slump cone tests, and slip resistance, as well as mechanical property tests including compressive, flexural, and tensile strength, and determination of elastic modulus. The obtained results showed a significant improvement in concrete properties, including a 45 % increase in flexural strength and a 62 % increase in tensile strength after adding polymer shot. These findings suggest that the addition of polymer shot can contribute to improving the properties of produced concrete, supporting sustainable resource management and waste minimization strategies.

# YUCOMAT Poster Presentations

### Influence of Common Catalysts on Curing Kinetics of Polyurethanes: Non-isothermal Rheological Method

<u>Mladen Timotijević</u><sup>1</sup>, Ivan Dimitrijević<sup>2</sup>, Danica Bajić<sup>1</sup> <sup>1</sup>Military Technical Institute, Belgrade, Serbia <sup>2</sup>Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia

This study investigates the influence of dibutyltin dilaurate (DBTDL) and ferric trisacetylacetonate (FeAA) on the curing kinetics of polyurethanes based on hydroxyl-terminated polybutadiene (HTPB) and polypropylene glycol (PPG) as prepolymers, and isophorone diisocyanate (IPDI) as the cross-linker. Rheological characteristics of samples with and without catalysts, including storage modulus (*G*'), loss modulus (*G*"), and complex viscosity ( $\eta^*$ ), were determined through non-isothermal conditions. The impact of these catalysts on the reaction kinetics was analyzed based on the observed changes in rheological properties. The investigation aimed to elucidate the effects of catalysts on the curing process of polyurethanes, providing insights into the mechanisms underlying their catalytic activity. The results contribute to a better understanding of the role of catalysts in controlling the kinetics of polyurethane curing reactions and the pot life of a mixture. These informationc are essential for optimizing the production and performance of composite materials in various applications, and are of special interest in advanced energetic materials for defense technology.

*Acknowledgement*: This work is supported by the Ministry of science, technological development and innovations (Serbia), Contract No. 451-03-66/2024-03/200325.

#### Optomagnetic imaging spectroscopy in human kidney cancer detection

<u>Aleksandra Dinić</u><sup>1</sup>, Lidija Matija<sup>1</sup>, Branislava Jeftić<sup>1</sup>, Ivana Stanković<sup>1</sup>, Gorana Nikolić<sup>2</sup> <sup>1</sup>Department of Biomedical Engineering, Faculty of Mechanical Engineering, University of Belgrade, Serbia <sup>2</sup>Institute of Pathology, Faculty of Medicine, University of Belgrade, Serbia

Kidney cancer is one of the 10 most common cancers in both men and women, accounting for between 3 and 4% of the total number of cancer patients. Current methods of determining cancer consist in observing the glass plates on which the kidney tissue is located, obtained by biopsy, fixed in paraffin, and using an optical microscope. The stage of the disease is determined by observing the appearance of the cells. There is a need to improve diagnostics, as well as automate the process of making diagnoses, in order to help doctors make a diagnosis. One possible way is the use of polarized light. This paper presents the use of optomagnetic imaging spectroscopy (OMIS) which showed high percentages of accuracy when detecting cervical, colon and oral cancer in earlier studies. The interaction of diffuse and polarized light with kidney tissue in the region of 450 to 750 nm normalized wavelength was examined. It has been shown that using light is possible to make a clear distinction between healthy and cancerous tissue, as well as to make a clear classification between low grade and high-grade samples. The interaction of polarized light with the sample gives a better classification of the result than the use of diffuse light. The clearest differences are observed when white polarized light and sample interact, in the regions between 450 and 500, as well as 500 and 570 nm normalized wavelength. The minimum differences in peak height, for the first region, are 14 442 units (healthy-cancerogenic tissue) and 6 546 units (also healthy-cancerogenic tissue), for the second region, providing a clear distinction between the normal-low grade-high gradecancerogenic tissue.

*Acknowledgement*: This work was funded by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia Grant No.: 451-03-47/2023-01/200007, February 3, 2023.

### Mechanochemical Synthesis of Ammonium-Iminodiacetato-Dithiocarbamate: An Environmentally Friendly Approach

<u>Slađana Kovačević</u><sup>1</sup>, Milica Kosović Perutović<sup>1</sup>, Marija Ristić<sup>2</sup>, Jana Mišurović<sup>1</sup>, Zorica Leka<sup>1</sup>

<sup>1</sup>University of Montenegro, Faculty of Metallurgy and Technology, Cetinjski put bb, 81000 Podgorica, Montenegro

<sup>2</sup>University of Kragujevac, Faculty of Science, Radoja Domanovića 12, 34000 Kragujevac, Serbia

Dithiocarbamates are a group of organic compounds that have a variety of agricultural, industrial, and medical applications. Ammonium-iminodiacetato-dithiocarbamate, (NH<sub>4</sub>)<sub>3</sub>idadtc, and its complexes with transition metals have shown fungicidal activity against the phytopathogenic fungus *Botrysphaeria dothidea*, which causes olive rot. Previously, (NH<sub>4</sub>)<sub>3</sub>idadtc was prepared using a traditional method which requires the use of significant amounts of methanol [1]. In order to optimize this method (shorter duration of synthesis, increased yield, avoiding the use of solvents), mechanochemical approach, recognized as "green chemistry", was studied.

The aim of this experimental work was to achieve a dithiocarbamate derivative of iminodiacetate,  $(NH_4)_3$ idadtc, through mechanochemical grinding in the planetary ball mill using zirconium oxide jars and balls. Iminodiacetate acid and ammonium-carbonate were grinded for 5 minutes, and after that CS<sub>2</sub> was added. IR spectra of the product were recorded at different reaction times of 1, 1.5, and 2 h. After their comparison, it was concluded that the reaction is completed within 1 hour. The product was characterized by elemental analysis, IR, and UV-Vis spectroscopy, which confirmed that the desired compound was obtained. This opens broad possibilities for eco-friendly, solvent-free synthesis of dithiocarbamate compounds.



#### **References:**

1. Leka, Z., Leovac, V., Lukić, S., Sabo, T., Trifunović, S., & Szécsényi, K. M. J. Therm. Anal. Calorim., 83(3) (2006) 687–691. doi:10.1007/s10973-005-6938-7

# Synthesis of highly porous Ti<sub>3</sub>AlC<sub>2</sub> MAX-phase resulting Ti<sub>3</sub>C<sub>2</sub> MXene with enhanced properties

Veronika Zahorodna<sup>1,2</sup>, Ivan Baginskiy<sup>1</sup>, Serhii Dukhnovskiy<sup>1</sup>, Veronika Kaurkovska<sup>1</sup>, Margaryta Potashna<sup>1</sup>, Stefano Ippolito<sup>3</sup>, Oleksiy Gogotsi<sup>1,2</sup>, Iryna Roslyk<sup>1,3</sup>, Yury Gogotsi<sup>3</sup> <sup>1</sup>Materials Research Centre Ltd., Kyiv, Ukraine <sup>2</sup>Y-Carbon Itd. (Carbon-Ukraine), Kyiv, Ukraine <sup>3</sup>Drexel University, Philadelphia, USA

MXenes, is a large family of 2D carbides and nitrides, that nowadays are among the most studied nanomaterials worldwide. They are mainly manufactured by selective wet-chemical etching of layered ceramics MAX-phases, ternary carbides and nitrides of early-transition metals that were initially developed for use in structural and high-temperature applications. The requirements for MAX-phases used as a precursor for MXenes differ drastically from those of structural MAX materials. However, MAX phase synthesis has not been optimized yet for MXene manufacturing. We develop highly porous Ti<sub>3</sub>AlC<sub>2</sub> (porosity about 70 %) from an inexpensive titanium sponge instead of a highly pure titanium powder and explain the mechanisms of reaction sintering and formation of porous MAX phase. MAX phase produced in such way can be easily ground into individual grains without time-consuming crushing and milling steps. Synthesis yield of Ti<sub>3</sub>C<sub>2</sub>Tx MXene from porous Ti<sub>3</sub>AlC<sub>2</sub> was 65 %. MXene obtained from this MAX phase, Ti<sub>3</sub>C<sub>2</sub>Tx, shows larger flake size and higher electrical conductivity up to 16 500 S/cm in thin films, compared to the materials produced from the costly fine titanium powder. The proposed approach may apply to the synthesis of other Ti-based and beyond-Ti MAX phases.

Acknowledgement: Supported by European Commission under HORIZON-Europe projects #101131147 "ESCULAPE", #101086184 "MX-MAP", #872370 "SALSETH".

### Role of Surface Terminations in MXene Thermodynamic Stability

Ervin Rems<sup>1,2</sup>, Yong-Jie Hu<sup>3</sup>, Yury Gogotsi<sup>3,4</sup>, Robert Dominko<sup>1,2</sup> <sup>1</sup>Department of Materials Chemistry, National Institute of Chemistry, Ljubljana, Slovenia <sup>2</sup>Faculty of Chemistry and Chemical Technology, University of Ljubljana, Ljubljana, Slovenia <sup>3</sup>Department of Materials Science and Engineering, Drexel University, Philadelphia, USA <sup>4</sup>A.J. Drexel Nanomaterials Institute, Drexel University, Philadelphia, USA

MXenes are a rapidly growing family of 2D transition metal carbides and nitrides that are promising for various applications, including energy storage and conversion, electronics, and healthcare. The family of MXenes has grown rapidly and the chemical space of synthesized MXenes has substantially expanded. The reported computational studies focus on -O and -F surface terminations or even assume non-terminated MXene surface. However, the synthesis of MXenes through molten salt etching or dry selective extraction (DSE) and chemical scissor-mediated structural editing of MXenes enables tuning of the surface chemistry of MXenes. To fill the gap between the experimental reality and theoretical predictions, we report a comprehensive screening for thermodynamically stable MXenes that accounts for the diverse surface chemistry of MXenes.

# Assessing the charge storage capability of hydrothermally treated biomass-derived activated carbon in different electrolyte formulations

<u>Minea Kapidžić</u><sup>1</sup>, Jana Mišurović<sup>1</sup>, Veselinka Grudić<sup>1</sup>, Milica Vujković<sup>2,3</sup> <sup>1</sup>University of Montenegro, Faculty of Metallurgy and Technology, Cetinjski put bb, Podgorica, Montenegro <sup>2</sup>University of Belgrade, Faculty of Physical Chemistry, Studentski trg 12-16, Belgrade, Serbia <sup>3</sup>Center for Interdisciplinary and Multidisciplinary Studies, University of Montenegro, Podgorica. Montenegro

Vine shoots were treated hydrothermally at 200 °C to investigate the sole effect of this carbonization method on pseudocapacitive behaviour (HTC) or synergy with the activating agent zinc chloride (HTCZnCl<sub>2</sub>). Hydrothermal treatment was followed by carbonization at 700 °C in the Ar atmosphere to achieve a higher degree of carbonization. The samples were investigated via cyclic voltammetry and electrochemical impedance spectroscopy in acidic, and alkaline electrolytes and in the series of neutral electrolytes (Li<sub>2</sub>SO<sub>4</sub>, Na<sub>2</sub>SO<sub>4</sub>, K<sub>2</sub>SO<sub>4</sub>). The addition of ZnCl<sub>2</sub> positively affects charge storage only at lower scan rates in alkaline and acidic medium. Unlike activated carbon, non-activated material showed an atypical capacitance-scan rate relationship, with a decrease at a low scan rate which is related to the competitive HER process. Better pseudocapacitive behavior was observed in neutral electrolytes for both materials. The highest specific capacitance (118 F g<sup>-1</sup> at 5 mV s<sup>-1</sup>) was measured for HTCZnCl<sub>2</sub> in saturated K<sub>2</sub>SO<sub>4</sub> which was chosen for the stability test in a symmetrical full-cell configuration.

Acknowledgment: This work is sustained by NATO Science for Peace and Security (SPS) Programme (project G5836-SUPERCAR). We thank the CEEPUS network for the mobility to the Institute of Chemical and Energy Engineering, University of Natural Resources and Life Sciences, Vienna, Austria.

# Exploring the potential of olive mill waste for the production of energy storage materials

<u>Kristina Lalatović</u><sup>1</sup>, Minea Kapidžić<sup>1</sup>, Sonja Kastratović<sup>1</sup>, Veselinka Grudić<sup>1</sup>, Milica Vujković<sup>2,3</sup>, Jana Mišurović<sup>1</sup> <sup>1</sup>University of Montenegro, Faculty of Metallurgy and Technology, Cetinjski put 2, Podgorica, Montenegro <sup>2</sup>University of Belgrade, Faculty of Physical Chemistry, Studentski trg 12-16, 11158 Belgrade, Serbia <sup>3</sup>Center for Interdisciplinary and Multidisciplinary Studies, University of Montenegro, Podgorica, Montenegro

The conversion of moist olive waste into high-performance electrodes for supercapacitors represents a significant step in sustainable technology. This promotes circular economy by valorizing materials into valuable resources, reducing waste, and supporting ecological innovation. To obtain activated carbon materials, we took olive mill waste, highly suitable for wet hydrothermal processing, and in the first step treated it hydrothermally at 200 °C. The second step was activation of the obtained hydrochar at 700 °C in an argon stream with two different activators (H<sub>3</sub>PO<sub>4</sub> and a mixture of Zn, Na, and K chloride salts). The synthesized materials were characterized structurally using FTIR and XRD methods, and their electrochemical behavior was tested by means of Cyclic Voltammetry in various aqueous electrolytes. Characterization showed that the material synthesized in the presence of H<sub>3</sub>PO<sub>4</sub> was pure carbon, while the one activated with chloride salts mixture contained impurities likely originating from metals present in the biomass. This was correlated with better charge storage performance of the H<sub>3</sub>PO<sub>4</sub>-activated carbon which delivered highest specific capacitance of 168 F g<sup>-1</sup> in 6 M KOH at a scan rate of 20 mV s<sup>-1</sup>. This research opens new possibilities of using an abundant industrial waste for high technology applications.

**Acknowledgement:** This research was supported by NATO Science for Peace and Security (SPS) Programme under grant G5836-SUPERCAR. Authors gratefully acknowledge the financial support from the bilateral project Montenegro-Slovenia "Biomass-derived carbons as anodes in sodium-ion batteries."

### Ambient pressure RWGS reaction: Advancements in reactor design and catalyst efficiency

<u>Dimitrij Ješić</u>, Blaž Likozar National Institute of Chemistry, Hajdrihova 19, 1001 Ljubljana, Slovenia

The conversion of  $CO_2$  into fuels and chemicals is crucial to minimize the negative impact of  $CO_2$  emissions on the environment. Although the direct use of  $CO_2$  is still emerging, syngas, mainly from coal gasification, remains the main source of CO and hydrogen for the chemical industry. The direct production of methanol and dimethyl ether from  $CO_2$  is challenging due to low yield and unfavorable thermodynamic conditions. The catalytic reverse water-gas shift reaction (RWGS) is a promising solution for the conversion of  $CO_2$  into fuels.

Recent advances in metal-based catalysts have significantly improved the efficiency, CO selectivity and stability of the RWGS reaction. Ongoing developments in catalyst design and a deeper understanding of the reaction mechanisms have led to these improvements. However, challenges remain, particularly with regard to catalyst stability at high temperatures and the precise identification of active reaction sites.

A significant advance in this field is the development of the XMTE (External Mass Transfer Eliminator) reactor. This reactor has been specifically designed to eliminate mass transfer limitations and thus allow accurate determination of microkinetic mechanisms and reaction kinetics. Such precise measurements are essential for the development of a microkinetic model and the determination of kinetic parameters. The XMTE reactor design represents a significant improvement over conventional CSTR reactors as it eliminates their limitations and allows for optimized operation.

In the present work, the RWGS reaction is investigated at ambient pressure using the HiFUEL W230 and CuZnGa catalyst. This serves as a starting point for further research into more complex conversions, such as oxidative methane coupling. The results provide valuable insights into increasing the efficiency and production of synthesis gas to fuels as well as the economics of the process. Overall, the XMTE reactor and the proposed process highlight the potential to address the global shortage of chemicals for the production of fuels and increase production efficiency.

Acknowledgment: The authors gratefully acknowledge the Slovenian Research Agency (research core funding nr. J7-4638, Hybreed, P2-0012, and I0-0039).

# Impact of molybdenum disulfide morphology on catalytic activity for hydrogen evolution reaction

<u>Jelena Rmuš Mravik</u><sup>1</sup>, Blaž Belec<sup>2</sup>, Milica Prvulović<sup>1</sup>, Bojana Babić<sup>1</sup>, Tijana Pantić<sup>1</sup>, Jasmina Grbović Novaković<sup>1</sup>, Sandra Kurko<sup>1</sup>

<sup>1</sup>Center of Excellence for Hydrogen and Renewable Energy (CONVINCE), Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia <sup>2</sup>Materials Research Laboratory, University of Nova Gorica, Ajdovščina, Slovenia

Molybdenum disulfide ( $MoS_2$ ) is known as a suitable catalyst for hydrogen evolution reaction (HER), exhibiting varying catalytic efficiencies depending on its structural characteristics such as edge sites, defects, and layer stacking. The catalytic activity of  $MoS_2$  is profoundly influenced by its morphology. Different forms such as nanosheets, nanoflowers, or nanotubes possess distinct surface areas, exposed active sites, and electronic properties, all of which play crucial roles in determining the catalytic performances of the material. Specific  $MoS_2$  morphologies can be easily achieved via hydrothermal synthesis that enables tailoring of desired properties of material by varying parameters of synthesis.

This study shows how specific morphological features such as edge sites, defects, and layer stacking affect catalytic performance for HER. Through a combination of different synthesis parameters such as precursors, time and temperature, the impact of different  $MoS_2$ morphology, including flower-like and flake-like structures on the catalytic activity of material is compared. Utilizing scanning electron microscopy different morphologies are identified, while x-ray diffraction confirmed the presence of hexagonal  $2H-MoS_2$  phase in both synthesized materials. The electrochemical activity of the material was tested with linear sweep voltammetry, cyclic voltammetry and electrochemical impedance spectroscopy. All measurements were performed in  $0.5 \text{ M H}_2\text{SO}_4$ . The results showed that both synthesized materials exhibit better catalytic activity compared to commercially available MoS<sub>2</sub>, achieving higher current densities for the same value of overpotential. In addition, flower-like structures that consist of nanosheet petals tend to exhibit superior HER activity compared to flake-like morphology, with the decrease of overpotential needed to achieve current density of 10 mA/cm<sup>2</sup> and lower charge transfer resistivity. Flower-like  $MoS_2$ , thanks to their specific morphology, exhibit abundant edge sites, indicating the importance of both the number of sites, but also their availability to the electrolyte, for improvement of catalytic activity.

*Acknowledgments:* This research was supported by the Science Fund of the Republic of Serbia, GRANT No. 14145 – PolyHER and NATO SPS GRANT G6037.

## P.S.I.C.2 Correlation between photoluminescence and photocatalytic properties of novel down and up-converting phosphors

<u>Tijana Stamenković</u>, Vesna Lojpur

Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Vinča, Belgrade, Serbia

The aim of this research was to investigate photoluminescence and photocatalytic properties of newly synthesized nanostructural phosphors. We prepared down-converting  $SrGd_2O_4$  doped with  $Dy^{3+}$  ions (1, 3, 5 and 7 at.%), and up-converting  $SrGd_2O_4$  co-doped with different concentrations of  $Yb^{3+}$  ions (2, 4, 6 at.%) and constant concentration of  $Ho^{3+}$  ions (1 at.%). Samples were prepared via combustion route, where formed gel was firstly burned at 500 °C for 1.5 h and then calcined at 1000 °C for 2.5 h. X-ray diffraction measurements indicated that all samples crystallize as a single phase with the orthorhombic lattice of  $SrGd_2O_4$  spinel. Scanning Electron Microscopy revealed irregularly shaped particles that form chain-like structures, with pores in between. Luminescent measurement showed presence of characteristic emission peaks related to  $Dy^{3+}$  or  $Ho^{3+}$  dopant ions. UV/Vis Diffuse Reflectance Spectroscopy was used to examine materials bandgap, and values of 4.3 eV were obtained for each sample, as well as the additional levels positioned in the gap. Photocatalytic activity was explored through the degradation reactions of selected organic dyes (Rhodamine B for down-convertors and Methylene Blue for up-convertors) under simulated solar irradiation. UV/Vis Absorption Spectroscopy was used to measure a decrease in dye concentration in water solutions. Aliquots of the working solutions were taken at the exact time intervals, and the results indicate a successful dye decomposition rate after 4 h. Also, obtained results suggest that samples with highest luminescence intensity demonstrated better photocatalytic activity, which implies great potential for as-synthesized powders to be used as multifunctional materials.

# The magnetic properties of CoFe<sub>2</sub>O<sub>4</sub> and CoFe<sub>2</sub>O<sub>4</sub>/SiO<sub>2</sub> prepared by thermal decomposition method

Ljubica Anđelković<sup>1</sup>, Marija Šuljagić<sup>1</sup>, Ana Mraković<sup>2</sup>, Vladimir Pavlović<sup>3</sup>, Marin Tadić<sup>2</sup> <sup>1</sup>University of Belgrade-Institute of Chemistry, Technology and Metallurgy, Department of Chemistry, Njegoševa 12, Belgrade, Serbia <sup>2</sup>"VINČA" Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of

Belgrade, Belgrade, Serbia <sup>3</sup>University of Belarade. Faculty of Aariculture. Nemaniina 6. Belarade. Serbia

The present study has dealt with the structural, morphological and magnetic properties of cobalt-ferrite ( $CoFe_2O_4$ ) and cobalt-ferrite in amorphous silica matrix ( $CoFe_2O_4/SiO_2$ ) prepared by thermal decomposition of appropriate acetylacetonate complexes. The synthesized materials were characterized with the use of X-ray powder diffraction (XRPD), scanning electron microscopy (SEM), electron dispersive spectrum (EDS) and transmission electron microscopy (TEM). The presence of a single-phase cubic spinel structure was confirmed for both investigated powders. The synthesized particles are highly agglomerated as a consequence of their nanometric sizes and ferrimagnetic nature. The microstructure of the composite indicated spongy porous clusters with less pronounced agglomeration than that of bare cobalt-ferrite. Closer inspection of the EDS map revealed that the  $CoFe_2O_4$  nanoparticles were homogeneously dispersed over the silica matrix. The pure  $CoFe_2O_4$  sample consisted of spherically shaped agglomerates with the primary particles being evidently in the sub-100 nm range and mostly polygonal in shape. Magnetic measurements were conducted using a SOUID magnetometer. The introduction of a silica matrix led to a slight decrease in coercivity at room temperature. The saturation magnetization value for  $CoFe_2O_4$  was about 75 emu/g at ambient conditions. As expected, the silica matrix strongly influenced the magnetization of the material ( $\sim$ 7.7 emu/g). The obtained results show the perspective for possible applications in various technological areas.

#### Surface chemistry of hydrothermally treated GO and GO-based nanocomposites

Milica Pejčić<sup>1</sup>, Željko Mravik<sup>1</sup>, Danica Bajuk-Bogdanović<sup>2</sup>, Marija Grujičić<sup>1</sup>, Darija Petković<sup>1</sup>, Janez Kovač<sup>3</sup>, Zoran Jovanović<sup>1</sup> <sup>1</sup>Laboratory of Physics, Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia <sup>2</sup>Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia <sup>3</sup>Department of Surface Engineering and Optoelectronics, Jožef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia

Graphene oxide is one of the most promising materials in nanotechnology, especially in electrochemical energy storage due to its two-dimensional nature and interesting surface chemistry. In this study, we investigated the influence of hydrothermal treatment (HTT; 1, 4, 8 and 12 h at 180 °C) on graphene oxide (GO) and its nanocomposites with 12-tungstophosphoric acid (WPA) and 3.4.9.10-pervlenetetracarboxylic dianhydride (PTCDA). The weight ratio of WPA and PTCDA, in respect to GO, was 15 wt.%, each. Fourier-transform infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS), and temperature-programmed desorption (TPD) methods were used to study the surface and structural properties before and after HTT. The FTIR and XPS revealed characteristic bands of GO and its oxidation degree, respectively. Also, the FTIR confirmed the presence of WPA and PTCDA in the nanocomposites. Upon hydrothermal treatment, it was concluded that HTT does not affect the structure of PTCDA. while a significant decrease in the number of oxygen functional groups was noticed, with complete elimination of epoxy groups for all investigated samples. By comparing the amount of desorbed groups (CO+CO<sub>2</sub>) from pristine GO, GO/WPA, GO/PTCDA and GO/WPA/PTCDA, it was concluded that in respect to pure GO, WPA does not influence evolution of groups from hydrothermally treated GO/WPA and has slightly reducing effect on GO/WPA/PTCDA. On the other hand, the addition of PTCDA led to an increased number of desorbed groups. The results indicate that HTT in combination with WPA and PTCDA can be used for enhancing the surface chemistry of GO-based nanocomposites. This research offers new insights into GO. WPA, and PTCDA interactions which may have useful implications for the development of electrochemical supercapacitors.

**Acknowledgment:** This research was supported by the Science Fund of the Republic of Serbia, grant No. 6706, Low-dimensional nanomaterials for energy storage and sensing applications: Innovation through synergy of action – ASPIRE and by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (contract No. 451-03-66/2024-03/200017).

### Modified glassy carbon electrodes with Zn/Ga-substituted cobalt ferrite for electrochemical detection of gallic acid

<u>Marija Grujičić</u><sup>1</sup>, Milica Pejčić<sup>1</sup>, Danica Bajuk-Bogdanović<sup>2</sup>, Marko Jelić<sup>1</sup>, Zoran Jovanović<sup>1</sup>, Ivana Stojković Simatović<sup>2</sup>, Sonja Jovanović<sup>1</sup> <sup>1</sup>Laboratory of Physics, Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia <sup>2</sup>Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia

For the electrochemical detection of gallic acid, nanoparticles of cobalt ferrite (CoFe<sub>2</sub>O<sub>4</sub>, CFO) and zinc/gallium-substituted cobalt ferrite (Co<sub>0.5</sub>Zn<sub>0.5</sub>Fe<sub>2</sub>O<sub>4</sub>, CFO\_Zn and CoFe<sub>1.5</sub>Ga<sub>0.5</sub>O<sub>4</sub>, CFO Ga. respectively) were synthesized by the solvothermal method using dihydrocaffeic acid (DHCA) as a surfactant. To modify surface groups, additional annealing at 450 °C in air was performed. All samples demonstrate diffraction maxima indicative of the cubic spinel phase by X-ray diffraction (XRD). The nanoparticles are non-agglomerated, spherical with an average size of 5±1 nm based on transmission electron microscopy (TEM). Fourier Transform Infrared Spectroscopy (FTIR) confirmed the presence of DHCA and showed that DHCA binds to the surface of the nanoparticles through carboxyl and catechol groups. Temperature-programmed desorption (TPD) analysis showed that almost all functional groups of CO disappear after annealing, while for CO<sub>2</sub> groups, the peak originating from carboxyl groups (~400 °C) decreases, but the peak from lactone groups (~600 °C) increases due to the influence of group recombination. The electrochemical properties were investigated by cyclic voltammetry (CV) with modified glassy carbon electrodes (m-GCE) prepared with CFO, CFO Zn, and CFO Ga nanoparticles. Cyclic voltammograms of all annealed samples exhibited good reversibility in the  $[Fe(CN)_{6}]^{3-/4-}$  electrolyte. The most efficient electron transfer was achieved when the mass ratio between the sample and Vulkan® was 85:15. The highest sensitivity towards gallic acid  $(10^{-4} \text{ M}, \text{ in Britton-Robinson buffer at pH 2})$  was attained using m-GCE with CFO\_Zn. The electrode was tested with three different concentrations of gallic acid: 10<sup>-3</sup>, 10<sup>-4</sup> and 10<sup>-5</sup> M and showed a positive response.

*Acknowledgments:* This research was supported by the Science Fund of the Republic of Serbia, grant No. 6706, Low-dimensional nanomaterials for energy storage and sensing applications: Innovation through synergy of action – ASPIRE and by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (contract No. 451-03-66/2024-03/200017).

#### Structural and magnetic properties of nanometric ε-Fe<sub>2</sub>O<sub>3</sub> prepared by microemulsion method

Marija Šuljagić<sup>1</sup>, Ljubica Anđelković<sup>1</sup>, Ana Mraković<sup>2</sup>, Vladimir Pavlović<sup>3</sup>, Marin Tadić<sup>2</sup> <sup>1</sup>University of Belgrade-Institute of Chemistry, Technology and Metallurgy, Department of Chemistry, Njegoševa 12, Belgrade, Serbia <sup>2</sup>"VINČA" Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia <sup>3</sup>University of Belgrade, Faculty of Aariculture, Nemaniing 6, Belgrade, Serbia

The aim of this study was to investigate the magnetic properties of novel  $\varepsilon$ -Fe<sub>2</sub>O<sub>3</sub>/SiO<sub>2</sub> composites prepared by the microemulsion method followed by programmed annealing treatment. The reverse micelle approach was applied using heptane and hexanol as the oil phase, respectively. The resulting powders were characterized using a range of experimental techniques and assessed for their magnetic properties. X-ray powder diffraction (XRPD) revealed pure  $\varepsilon$ -Fe<sub>2</sub>O<sub>3</sub> alongside amorphous SiO<sub>2</sub> in both cases. The nanometric nature of  $\varepsilon$ -Fe<sub>2</sub>O<sub>3</sub> particles uniformly incorporated into the SiO<sub>2</sub> matrix was confirmed by Scanning and Transmission Electron Microscopy (SEM and TEM). As a result of appropriate annealing treatment, the obtained materials possessed high coercivity values. The findings of this study give hope that with appropriate synthesis alterations, pure  $\varepsilon$ -Fe<sub>2</sub>O<sub>3</sub> with superior magnetic properties can be obtained which opens the way for its successful applications in technology.

#### P.S.I.D.1

# Surfactant-modified bentonites for the removal of nonsteroidal antiinflamatory drug: targeting ibuprofen

Danijela Smiljanić<sup>1</sup>, Aleksandra Daković<sup>1</sup>, Milena Obradović<sup>1</sup>, Milica Ožegović<sup>1</sup>, Marija Marković<sup>1</sup>, Milica Todorović<sup>2</sup> <sup>1</sup>Institute for Technology of Nuclear and Other Mineral Raw Materials, Belgrade, Serbia <sup>2</sup>University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia

Natural bentonites, owing to their hydrophilic surfaces, have limited affinity for the adsorption of anionic species and/or hydrophobic molecules. To address this limitation, bentonite can be modified by intercalating cationic surfactants into its interlayer regions through ion exchange with naturally occurring exchangeable cations. This process results in a transformation of the surface properties of bentonite from hydrophilic to hydrophobic due to the presence of surfactants within the interlamellar space. These newly acquired hydrophobic characteristics offer active sites for the adsorption of hydrophobic organic molecules.

This study aimed to prepare and characterize surfactant modified bentonites, and evaluate their efficacy in removal of ibuprofen sodium, a widely recognized water contaminant. Natural bentonite (Šipovo deposit, Bosnia and Herzegovina) was modified using surfactant (quaternary ammonium salt) under the tradename Arquad®2HT-75, at levels corresponding to 50 and 100 % of the bentonite's cationic exchange capacity. Zeta potential measurement and XRD analysis confirmed the presence of the surfactant in the prepared composites. Adsorption experiments demonstrated that the uptake of ibuprofen by the composites was rapid and increased with higher adsorbent mass, surfactant concentration, and initial pharmaceutical concentrations. These findings suggest that bentonite modified with surfactant could serve as an efficient adsorbent for the removal of ibuprofen from contaminated water sources.

#### P.S.I.D.2

#### Solid residue of pyrolysis of agricultural waste as an alternative fossil fuel

Emilija N. Vukićević<sup>1</sup>, Jelena N. Isailović<sup>2</sup>, Gordana Gajica<sup>3</sup>, Vesna Antić<sup>2</sup>, Mališa Antić<sup>2</sup>, Jan Schwarzbauer<sup>4</sup>, <u>Branimir Jovančićević</u><sup>1</sup> <sup>1</sup>University of Belgrade, Faculty of Chemistry, Studentski trg 12-16, 11000 Belgrade, Serbia <sup>2</sup>University of Belgrade, Faculty of Agriculture, Nemanjina 6, 11080 Zemun, Belgrade, Serbia <sup>3</sup>University of Belgrade, Institute of Chemistry, Technology and Metallurgy (IChTM), Njegoševa 12, Belgrade, Serbia <sup>4</sup>RWTH Aachen University. Lochnerstr. 4-20, 52056 Aachen, Germany

It started from the idea that waste from the processing of corn, tobacco and tomatoes can be used as a raw material for obtaining fuel. Bearing in mind that this material mainly contains compounds of a macromolecular structure, it was assumed that the process of dry distillation (pyrolysis) could be applied for this purpose, which involves heating without the presence of oxygen.

After the characterization of the waste biomass was done (hygroscopic moisture, ash, pH, elemental analysis, thermal power, thermogravimetric TG analysis), pyrolysis was applied at 400 and 500 °C, lasting 5, 15 and 30 minutes. Pyrolysis was done on two furnaces: a smaller one, MTF 10/15/130, Carbolite, UK and a larger one, Nabertherm, Kompakt Rohrofen RD, 30/200/11.

Since the gaseous and solid phases were separated, the solid residue was characterized and analyzed in detail. It was first rinsed with acetone and air-dried. Physical-chemical characterization of the solid residue included determination of moisture content, ash, pH, determination of heat capacity, elemental analysis, Inductively Coupled Plasma (ICP), Fourier-transform infrared spectroscopy (FTIR), Brunauer–Emmett–Teller (BET) and scanning electron microscopy (SEM) analysis.

The obtained results were compared with similar results for wood and different types of coal (peat, lignite, brown coal, hard coal and anthracite). The best fuel characteristics were shown by the corn solid residue obtained by pyrolysis at 400 °C, during 30 minutes in a smaller furnace.

*Acknowledgment*: These researches were carried out as part of a AGRIPLAST project, funded by Germany Federal Ministry of Education and Research.

### P.S.I.D.3

# Investigation of various catalytic materials for heterogeneous conversion of biomass-derived glycolic acid

<u>Aleksa Kojčinović</u><sup>1</sup>, Florian Harth<sup>1,2</sup>, Blaž Likozar<sup>1</sup>, Miha Grilc<sup>1</sup> <sup>1</sup>Department of Catalysis and Chemical Reaction Engineering, National Institute of Chemistry, Ljubljana, Slovenia <sup>2</sup>Institute of Chemical Technology, Universität Leipzig, Leipzig, Germany

Glycolic acid (GA), an  $\alpha$ -hydroxycarboxylic acid, is a bifunctional molecule primarily used as a precursor for biopolymers and also shows significant potential as a platform chemical. It can be obtained from biomass through various biotechnological or catalytic processes. Recently, extensive research has focused on upgrading GA via heterogeneously catalyzed hydrogenation reactions. Catalysts such as ruthenium, platinum, palladium, and other supported metals have demonstrated high potential, achieving conversions and selectivity rates over 90 % for the production of bio ethylene glycol (EG). EG is an important biopolymer precursor and serves as an additive in various consumer products, including antifreeze, brake fluids, cosmetics, solvents, and paints.

This study will provide a detailed investigation of the reaction mechanism for the hydrogenation of biomass-derived glycolic acid to ethylene glycol using various carbon-supported noble-metal catalysts, examining all intermediates and potential reaction pathways. The study will explore reactions involving hydrogenation, deoxygenation, and decarboxylation under different reaction conditions and catalysts, thoroughly describing their correlations. Additionally, it will define the microkinetic model used to describe the three-phase system (gas-liquid-solid) encompassing all the heterogeneous reactions involved.

Acknowledgments: Authors gratefully acknowledge financial support provided by the European Union/European Regional Development Fund (EU/EFRE) via Sächsische Aufbaubank – Förderbank (SAB) project 100300939 and from the European Commission (e-CODUCT). Moreover, funding from the German Academic Exchange Service (DAAD) for bilateral exchange project 57450888 and from Slovenian Research Agency (ARRS) for bilateral exchange project BIDE/19-20-001 is acknowledged, as well as the funding from ARRS via Research Program P2-0152.

#### New approach of thin MXene coating for PCL membrane

<u>Yevheniia Husak</u><sup>1,2</sup>, Yuliia Varava<sup>1,2</sup>, Natalia Waloszczyk<sup>2</sup>, Viktoriia Korniienko<sup>1,3</sup>, Kateryna Diedkova<sup>1,3</sup>, Volodymyr Deineka<sup>1,3</sup>, Veronika Zahorodna<sup>4</sup>, Oleksiy Gogotsi<sup>4</sup>, Wojciech Simka<sup>2</sup>, Maksym Pogorielov<sup>1,3</sup> <sup>1</sup>Sumy State University, Sumy, Ukraine <sup>2</sup>Silesian University of Technology, Gliwice, Poland <sup>3</sup>University of Latvia, Riga, Latvia <sup>4</sup>Materials Research Center LTD, Kyiv, Ukraine

Polycaprolactone (PCL) electrospun membranes are widely used for the development of tissueengineering constructions due to high biocompatibility and controllable biodegradation. Recently, gold- and graphene-based PCL scaffolds were successfully used for conductive tissue regeneration (hear, nerve tissue), but low biocompatibility required more advanced strategies to improve clinical outcomes. There are several publications with successful application of 2D nanomaterials, MXenes (Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>), for PCL electrospun mats modifications. Different strategies (alkali and acidic pretreatment, oxygen plasma) are used to facilitate the MXene deposition of hydrophobic PCL membrane. To provide uniform MXene distribution over the electrospun PCL membrane, we aimed to develop alcohol-assisted deposition technology.

PCL electrospun membrane was immersed twice into alcohol-based  $Ti_3C_2T_x$  MXene solution (96% ethanol containing 200 mg ml<sup>-1</sup> MXene) for one hour with 24 hours drying at room temperature. Scanning electron microscope (SEM), energy-dispersive X-ray analysis (EDX) and Contact angle measurement were used to assess structural and elemental composition of asspun and MXene-deposited PCL mats. Additionally, biocompatibility assay was used to prove a safety profile of novel construction.

Our research allows us to provide uniform distribution of MXenes over the electrospun PCL membrane with deep penetration of 2D sheets. Alcohol-assisted deposition allows to reduce possible deposition of alkali or acid remnants and provide electrical conductivity for specific tissue regeneration purposes.

**Acknowledgement**: This research received support from the Horizon Europe MSCA-2021-SE-01 project 101086184 MX-MAP and from the Ukraine MES grant ID: 0122U000784. Electrospun fibres provided under the bilateral LV-UA projects "Implementation of 2D bi-layered nanomembranes for guided tissue regeneration in endo-perio lesions and periimplantitis" and "Novel copper-loaded wound healing patches with advanced regeneration capacity and antibacterial effect".

### MXene-based antifungal photothermal ablation

<u>Valeriia Korniienko</u><sup>1</sup>, Yuliia Varava<sup>1</sup>, Veronika Zahorodna<sup>3</sup>, Oleksiy Gogotsi<sup>3</sup>, Viktoriia Korniienko<sup>1,2</sup>, Maksym Pogorielov<sup>1,2</sup> <sup>1</sup>Sumy State University, Sumy, Ukraine <sup>2</sup>University of Latvia, Riga, Latvia <sup>3</sup>CARBON-UKRAINE Ltd., Kiev, Ukraine

Fungal infections present an ongoing challenge to global public health, caused by the emergence of drug-resistant strains. MXene nanosheets showed antifungal properties by inhibiting mycelium and spore germination due to physical damage to the cells [1]. Since MXene exhibits photo-thermal activity, it has been hypothesized that one of the processes behind its biocidal activity is its ability to kill microorganisms by photothermal means when exposed to light. MXenes, activated by near-infrared (NIR) laser light, convert it into heat, effectively targeting microorganisms. This mechanism heats microbes while enhancing MXene's ability to disrupt fungal cells [2].

Our study aims to determine the most effective laser mode for MXene-based photothermal therapy in combating drug-resistant fungal infections.

 $Ti_3C_2$  MXene was evaluated as a photothermal agent against Candida albicans at an initial concentration of 10<sup>5</sup> CFU/mL using MXene suspensions in a concentration of 50 µg/mL. Fungal suspension with MXene was cultured and exposed by laser (continuous mode, 2 watts, 10 Hz) for 10 minutes. Evaluation of colony-forming units (CFU/mL) was conducted after 24-hour incubation at 37 °C compared to untreated controls.

Temperature changes were monitored to evaluate photothermal conversion, assessing its antifungal activity through growth inhibition assays. Applied MXene concentration, NIR laser intensity, and exposure duration were optimal to provide the photothermal effect against fungal strain, leading to the complete eradication of fungal cells.

The obtained results for Candida albicans can be used for the establishment of standardized procedures for MXene's photothermal ablation against different fungal species aimed at achieving optimal photothermal effects.

*Acknowledgment*: This research received support from Horizon Europe projects MX-MAP (#101086184) and ESCULAPE (#101131147).

### **References:**

- 1. Gim Pao Lim et al. Ceramics International, 46 (2020) 20306.
- 2. S. Yougbaré, et al. Nanomaterials (Basel), 10 (2020) 1123.

### P.S.II.A.5

### Immobilization of yeast cells in biopolymer systems using freeze-drying technique

<u>Nataša Obradović</u><sup>1</sup>, Bojana Balanč<sup>2</sup>, Vukašin Ugrinović<sup>2</sup>, Verica Đorđević<sup>1</sup>, Nemanja Stanisavljević<sup>3</sup>, Mina Volić<sup>2</sup>, Viktor Nedović<sup>4</sup>

<sup>1</sup>University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11000 Belgrade, Serbia <sup>2</sup>University of Belgrade, Innovation Center of Faculty of Technology and Metallurgy, Karnegijeva 4, 11000 Belgrade, Serbia

<sup>3</sup>University of Belgrade, Institute of Molecular Genetics and Genetic Engineering, 11000 Belgrade, Serbia <sup>4</sup>University of Belgrade, Faculty of Agriculture, Nemaniina 6, 11080 Beograd, Serbia

The application of advanced yeast cell immobilization techniques has significantly enhanced beer production processes. This study aimed to immobilize yeast cells (*Saccharomyces pastorious*) in alginate-based carriers using the freeze-drying technique. For this purpose, medium-viscosity sodium alginate was utilized. After lyophilization, the resulting powders were analyzed for cell viability, storage stability, particle size, and moisture content. Morphological characteristics were examined using scanning electron and optical microscopy. The low moisture content in the obtained powders indicates that these types of systems are microbiologically stable. The average diameter of immobilized yeast cells was larger than that of non-immobilized cells, measuring 7.33 $\pm$ 0.97 and 3.21 $\pm$ 0.39 µm, respectively. Surface charge analysis confirmed the physicochemical stability of the immobilized cell systems, showing a negative surface charge. The low surface charge of free cells indicated a tendency to aggregate, as confirmed by optical microscopy. SEM micrographs showed successful cell immobilization in the carriers. The study concludes that the freeze-drying technique is effective for yeast cell immobilization and suitable for industrial applications, offering high productivity and maximum cell protection.

Acknowledgment: This work was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (Science and Technology Development Programe–research projects of the Republic of Serbia and the People's Republic of China, Contract No. 451-02-1236/2023-05).

#### P.S.II.A.6

### *In situ* incorporation and calcination of Zn-Al LDH during PEO processing in close to neutral pH electrolytes

<u>Kristina Mojsilović</u><sup>1</sup>, Maria Serdechnova<sup>2</sup>, Carsten Blawert<sup>2</sup>, Mikhail L. Zheludkevich<sup>2,3</sup>, Stevan Stojadinović<sup>1</sup>, Rastko Vasilić<sup>1</sup> <sup>1</sup>University of Belarade, Faculty of Physics, Studentski tra 12-16, 11000 Belarade, Serbia

<sup>2</sup>Institute of Surface Science, Helmholtz-Zentrum Hereon, Max-Planck-Straße 1, 21502 Geesthacht, Germany

<sup>3</sup>Institute of Materials Science, Faculty of Engineering, Kiel University, Kaiserstraße 2, 24143 Kiel, Germany

Utilizing elevated voltages that induce dielectric breakdown of the initial oxide film on valve metals such as Al, Mg, Ti, etc., plasma electrolytic oxidation (PEO) facilitates the creation of oxide coatings exhibiting excellent adhesion, thermal and electrical properties, as well as corrosion and wear resistance. The integration of appropriate particles into PEO coatings can additionally be used in order to add functional properties to the coatings, for example enhancing their photocatalytic properties. One of the potential functional particulate materials is layered double hydroxide (LDH). In this research, PEO process was employed for preparing oxide-based coatings on AA2024 aluminum alloy in electrolytes containing Zn-Al LDH particles. Sodium hexametaphosphate aqueous solution was selected as the standard electrolyte, based on its almost neutral pH value considered as important for the stability of LDH in the electrolyte. Different additives to the standard electrolyte were examined including 2-mecaptobenzothiazole (MBT) and different Zn-Al LDH compounds: LDH[MBT], LDH[CO<sub>3</sub>] and  $LDH[CO_3]+MBT$ . Formed coatings were characterized with respect to their morphology, phase and chemical composition, photocatalytic activity and corrosion protection properties. Coating thickening and compactness evolution were noted for all coatings with LDH additions to the standard electrolyte. Obtained coatings are well-crystallized featuring  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> and two Zn-containing crystalline phases ZnO and NaZnPO<sub>4</sub> originating mainly from the LDH addition to the electrolyte. PEO coatings formed in this study demonstrated very reasonable photocatalytic activity for immobilized photocatalysts, reaching 52 % after 6 h under UV irradiation. Zn-Al LDH addition improved the impedance modules at low frequencies for two orders of magnitude compared to the bare AA2024 alloy immersed in 3.5 % NaCl.

#### P.S.II.A.7

# Crack growth and deformation monitoring in additively manufactured pipe ring specimens using contactless measurement

<u>Isaak D. Trajković</u><sup>1</sup>, Miloš S. Milošević<sup>1</sup>, Aleksandar S. Sedmak<sup>2</sup>, Zoran M. Radosavljević<sup>3</sup>, Bojan I. Međo<sup>4</sup>

<sup>1</sup>Innovation center of the Faculty of Mechanical Engineering in Belgrade, Kraljice Marije 16, 11000 Belgrade, Serbia

<sup>2</sup>University of Belgrade, Faculty of Mechanical Engineering, Kraljice Marije 16,

11000 Belgrade, Serbia

<sup>3</sup>Research and Development Institute Lola, 70A Kneza Viseslava Street, 11030 Belgrade, Serbia <sup>4</sup>University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11000 Belgrade, Serbia

In engineering practice, the integration of additively manufactured parts is becoming common. These parts serve both as temporary functional components within larger assemblies and, increasingly, as permanent replacement parts that effectively replace original parts. Evaluating the fracture resistance of these models is essential because of their frequent interaction with other assembly parts or exposure to external loading, which could compromise their structural integrity. In this work, a new geometry of specimens for fracture examination of pipeline materials is performed on additively manufactured sample. The tests were carried out on pipe ring tensile specimens using a Shimadzu AGS-X universal testing machine (100 kN) and a specially designed tool for cylindrical specimens, in correlation with Aramis 2M Digital Image Correlation System (DIC). The specimens were produced on a EOS Formiga P100 printer from polyamide polymer (PA12) with 100 % infill. A stress concentrator (sharp notch) is fabricated along the longitudinal direction being exposed to forces which act in the hoop direction, mimicking the internal pressure in the pipeline. DIC was used to measure the crack opening displacement (CMOD), crack tip opening displacement (CTOD), crack length ( $\Delta a$ ) and, in general, displacement and strain fields. It is concluded that adequate and reproducible results have been obtained by using this technique.

Acknowledgment: The work was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (contracts No. 451-03-66/2024-03/200213 and 451-03-65/2024-03/200135).

#### Measurement Techniques for Dissolution of Solid Metal in Liquid Metal

<u>Krzysztof Kania</u><sup>1</sup>, Grzegorz Zając<sup>1</sup>, Jan Kudláček<sup>2</sup>, Dariusz Buchczik<sup>1</sup>, Jiří Kuchař<sup>2</sup>, Franciszek Berger<sup>3</sup> <sup>1</sup>Silesian University of Technology, Faculty of Automatic Control, Electronics and Computer Science, Gliwice, Poland <sup>2</sup>Czech Technical University, Faculty of Mechanical Engineering, Prague, Czech Republic <sup>3</sup>Rockwell Automation sp. z o.o, Warszawa, Poland

Intensive dissolution of solid metals or their alloys in liquid metals is a phenomenon occurring in many production processes, mainly in metallurgy, foundry, nuclear technology, as well as in the hot dip galvanizing process. Dissolution in liquid metals is a complex process and depends on many physicochemical phenomena, including interfacial reactions. The hypothetical mechanisms of dissolution of solid metals in liquid metals assume that the transport of solid metal atoms into the liquid takes place via the intermetallic layer and that the entire dissolution process is controlled by diffusion in the solid state. Determination of the dissolution rate is necessary to predict the formation of coatings obtained by the hot dip method and to select materials for work in contact with liquid metals.

The article analyzes the current state of knowledge on the mechanisms of dissolution of solid metals in liquid metals. It was found that the most objective results of the dissolution rate are provided by methods in which the dissolution takes place as a result of mass transfer phenomena and no intermetallic layers are formed on the surface, which may disturb the dissolution process. For this purpose, assumptions have been developed for the construction of a universal dissolution test stand using the rotating disk method. Dissolution tests of steel with various Si contents in a zinc bath was carried out on a prototype test stand. The growth kinetics and structure of the coatings obtained under stationary conditions in the traditional hot dip galvanizing process were determined on the tested steels. It was found that at a disk rotation speed of 200 rpm, no intermetallic layer was formed on the steel surface and that further increasing the disk rotation speed did not affect the dissolution rate. The intensity of dissolution of steel in the zinc bath increases with the increase of Si in the steel up to 0.05 wt.%. Higher Si contents in steel reduce the intensity of dissolution of steel in liquid zinc. The obtained dissolution results are in correlation with the thickness of intermetallics formed in the coating under stationary conditions.

# Prediction and synthesis of low-work-function graphene nanostructures intercalated by alkali metals

<u>Yevhen Len</u><sup>1,2</sup>, Mykhailo Varvarin<sup>1,2</sup>, Vitalii Lebed<sup>1,2</sup>, Oleh Feia<sup>1,2</sup>, Oksana Lisova<sup>1,3</sup>, Iryna

Galstian<sup>1</sup>

<sup>1</sup>G.V. Kurdyumov Institute for Metal Physics of NASU, Kyiv, Ukraine <sup>2</sup>Kyiv Academic University, Kyiv, Ukraine <sup>3</sup>Chuiko Institute of Surface Chemistry of NASU, Kyiv, Ukraine

The work function (WF) of electrons in various materials is one of the most important parameters that determine the operating ability and energy efficiency of many products in electronics, electrical engineering, and energy. Modern nanotechnologies and nanomaterials have opened up the ways to obtain systems with predetermined work function values, including small ones. The present work is devoted to the theoretical prediction, by means of *ab initio* DFT calculations, of the structure and electronic properties of model low work function materials based on bilayer graphene (BGr) intercalated with alkali metals (AMs). We also present the results of the experimental study of the structure and electronic properties of similar graphene nanostructures electrochemically deposited on nickel and silicon substrates with and without intercalation with alkali metals.

For DFT calculations we used the Quantum Espresso software package. Calculations were performed using the PBEsol functional, dipole compensation, and Van der Waals correction. Relaxation was applied to all structures. Our study shows that intercalation of BGr makes the AA configuration more stable than typical for pure BGr the AB configuration (*i.e.* a phenomenon of AA type BGr stabilization is observed). Calculated WF values for the studied structures show a significant decrease in WF for BGr with AM-O-AM dumbbells where one AM atom is fixed between graphene layers.

The stable graphene films (GFs) are formed from multilayer graphene flakes by electrochemical deposition on substrates. The electrochemical method is also used to carry out the AM (rubidium) atoms adsorption on the surface and their intercalation between the near-surface graphene layers. The SEM with EDX and Raman spectroscopy are used to study the presence of adsorbed and intercalated AM atoms. The Raman spectra were obtained using a laser with wavelength of 532 nm. The pure and intercalated GFs demonstrate the main peaks attributed to the multilayer graphene. The fitting of the main peaks and the comparison of their main parameters (position of centre, height, width at half height) allowed us to identify the electron doping and the deformation of the GFs due to the intercalated atoms fixed between the near-surface graphene layers.

#### 25<sup>th</sup> YUCOMAT 2024 & XIII WRTCS Herceg Novi, September 2 - 6, 2024

P.S.II.B.7

## Kinetics of positive ions in H<sub>2</sub> gas

Željka Nikitović, Zoran Raspopović Institute of Physics University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

Transport parameters of species in gas plasma are of great importance for understanding the nature of molecular and ionic interactions in gas. These properties include mean energy, drift velocity, diffusion coefficients, ionization and chemical reaction coefficients, chemical reaction coefficients for ions, and (rarely) excitation coefficients, and are very useful in the chemical industry for the design of many types of transport and process equipment. Hydrogen, the first element of the periodic table, is one of the most common elements on Earth and in its gaseous form is a fuel for obtaining energy. Hydrogen is a highly explosive gas and produces one of the highest flame temperatures. They serve us to get energy, communicate, protect and build the body.

Given the current interest in liquid and/or liquid models in gas, data on swarm coefficients for positive and negative ions for hybrid and fluid codes are needed. Atmospheric and near-atmospheric pressure glow discharges generated in both pure hydrogen and hydrogen-air mixtures have been studied using a plasma chemistry code originally developed for simulations of electron-beam-produced air plasmas.

*Acknowledgments*: The authors acknowledge funding provided by the Institute of Physics University Belgrade, through the grant by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia.

## Adsorption-desorption processes on polymer-carbon coatings for solar energy collectors

Mykola Shevchenko, <u>Iryna Galstian</u>, Yulia Bozbey, Mykhailo Rud, Evgen Len G.V. Kurdyumov Institute for Metal Physics, N.A.S. of Ukraine, 36 Academician Vernadsky Boulevard, UA-03142 Kyiv, Ukraine

This work is devoted to the preparation of heat-resistant polymer-carbon coatings (PVDF+25 wt.% MWCNT) on a copper substrate. The kinetic processes of adsorption-desorption of the residual atmosphere molecules were studied during external contactless heating by the radiation of a reflector lamp and subsequent cooling of the electrode after switching off the light source.

The sample, in the form of a copper plate with a diameter of 84 mm and a thickness of 28 mm, with an internal cavity, the volume of which was 110 cm<sup>3</sup>, was placed in a vacuum chamber with a quartz glass window. The internal cavity increased the adsorption area by almost 4 times (up to 200 cm<sup>2</sup>), allowed it to fill it with gaseous impurities of the residual atmosphere and, most importantly, almost completely reduced the dissipation of thermal energy released during adsorption. The sample was heated to a temperature of 85-180 °C by a conventional 60 W incandescent reflector lamp from the side of the quartz glass. The method is based on non-contact heating of the sample and temperature measurement with a chromel-alumel thermo-couple. During the research, the dependence of the sample temperature on the irradiation time was measured during the heating process, and after turning off the light source, the dependence of the temperature on the cooling time of the sample was measured during the heat loss due to thermal conductivity.

The developed coating allows to reach temperatures up to 190 °C in vacuum. At the same time, the effects of adsorption-desorption of gases on the surface of the composite material PVDF+25 wt.% BWNTs play a significant role both in the process of its heating and after switching off the light source. In addition, a significant and prolonged increase in the temperature of the sample is observed after switching off the light source due to the adsorption of molecules from the residual atmosphere. The lower the maximum temperature of the sample, the more pronounced the collector heating effect after the light source is turned off, and the longer it takes for the system to return to the initial state (light-off temperature).

The effect of adsorption heating of the collector is well reproducible in subsequent cycles of heating-cooling of the sample and can be used in solar energy collectors to combine light absorption with additional energy accumulation in them due to physical adsorption.

### Zn-species containing oxide coatings: photocatalysts vs. adsorption

<u>Nenad Tadić</u><sup>1</sup>, Kristina Mojsilović<sup>1</sup>, Srna Stojanović<sup>2</sup>, Ljiljana Damjanović-Vasilić<sup>2</sup>, Stevan Stojadinović<sup>1</sup>, Rastko Vasilić<sup>1</sup>

<sup>1</sup>University of Belgrade, Faculty of Physics, Studentski trg 12-16, 11000 Belgrade, Serbia <sup>2</sup>University of Belgrade, Faculty of Physical Chemistry, Studentski trg 12-16, 11000 Belgrade, Serbia

Mixed Zn-species containing oxide coatings are prepared by conventional DC plasma electrolytic oxidation (PEO) of aluminum in water solution of boric acid and borax, with addition of Zn-loaded 13X synthetic zeolite. In addition, a set of oxide coatings with co-deposited ZnO nanoparticles and 13X zeolite from the same electrolyte is prepared. Scanning electron microscopy equipped with energy dispersive X-ray spectroscopy, X-ray diffraction and AFM imaging are employed to monitor the morphological, structural, and chemical changes of obtained oxide coatings. It was found that chemical and phase compositions strongly depend on PEO time. Photoluminescence and photodegradation of methyl orange served as a tool to estimate the potential application of the obtained coatings. Photoluminescence measurements showed that clearly observable bands inherent to  $Al_2O_3$  and ZnO are present in the formed coatings. The study showed that adsorption of methyl orange and its photodegradation under simulated sunlight are competing processes.

# Impact of the hybrid graphene-dielectric metasurface resonant oscillations on the propagation properties of surface plasmon-polaritons using simulation techniques

Z. E. Eremenko Usykov Institute for Radiophysics and Electronics NASU, Kharkiv, Ukraine

We propose a method to enhance and modify the surface plasmon-polariton (SPP) propagation length by designing a resonant metamaterial with an effective near-zero refractive index (ENZRI) regime at resonant frequencies, intended for use as a substrate for graphene.

Through simulations in Comsol Multiphysics software, we investigated the propagation of SPP in a graphene layer enclosed between two homogeneous dielectric media (air and ENZRI material) when excited by an electromagnetic plane wave. Our results confirmed that such a substrate indeed enhances the SPP wavelength and SPP propagation length in graphene.

To achieve the ENZRI regime in the graphene substrate, we propose utilizing a resonant alldielectric metasurface, conceptualized as a 2D photonic crystal (PC). The effective permittivity and permeability of the PC were calculated near the Dirac point frequency using effective medium theory, confirming the presence of ENZRI for a 2D PC consisting of silicon disks and an air substrate. Moreover, we demonstrated that a 3D PC with corresponding dielectric rods reduces to a 2D metasurface for rod heights above  $2\lambda$ . Consequently, the ENZRI results from the 2D metasurface unit cell model can be applied to the 3D model with considerably long rods. There is maximum electromagnetic absorption near the resonant frequency owing to losses in graphene layer. Similar results have been obtained with dielectric spheres. Such an absorption it is possible to evident about SPP propagation in graphene layer.

### CFD study of magnetic hysteresis heating in monolith reactor

<u>Andraž Pavlišič</u><sup>1</sup>, Anja Sedminek<sup>2</sup>, Sašo Gyergyek<sup>2</sup> <sup>1</sup>National Institute of Chemistry, Hajndrihova 19, 1000 Ljubljana, Slovenia <sup>2</sup>Jozef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia

Magnetic hysteresis heating is a phenomenon where magnetic materials experience temperature rise due to cyclic magnetization and demagnetization. This effect has practical implications in various applications, including induction heating and magnetic hyperthermia. Computational fluid dynamics (CFD) plays a crucial role in understanding and optimizing this process [1,2].

*Hysteresis Characterization*: We experimentally analyze the hysteresis behavior of a magnetic system. The monolith structure, purged with hydrogen gas, experiences cyclic magnetization and demagnetization. Our goal was to quantify the resulting temperature rise and understand its impact on reactor performance.

**CFD Simulations**: Using CFD simulation, we model the fluid flow and heat transfer within the reactor. The monolith's magnetic properties are incorporated into the simulations. We investigate how hysteresis affects the temperature distribution and overall efficiency.

**Optimization Strategies:** Based on CFD results, we propose optimization strategies to exploit hysteresis-induced heating. Adjustments to fluid flow rates, reactor geometry, and magnetic material properties were explored. Our goal was to enhance reactor performance while managing temperature distribution.

*Experimental Validation*: We validate our CFD predictions through experimental tests. The monolith reactor is subjected to varying magnetic fields, and temperature measurements were taken. Comparisons between simulations and experiments provided insights into hysteresis effects.

In summary, our research contributes to understanding and controlling magnetic hysteresis heating in fluid reactors with monolith structures. By combining experimental data and CFD simulations, we aim to optimize reactor design for efficient and safe operation.

#### **References:**

1. M. R. Almind et al., ACS Appl. Nano Mater., vol. 4, no. 11, pp. 11537–11544.

2. M. G. Vinum et al., Angew. Chemie, vol. 130, no. 33, pp. 10729-10733.

### High–Entropy Oxides: A New Frontier in Photocatalytic CO<sub>2</sub> Hydrogenation

Igor Djerdj<sup>1</sup>, Dalibor Tatar<sup>1</sup>, Habib Ullah<sup>2</sup>, Mohit Yadav<sup>3</sup>, Jelena Kojčinović<sup>1</sup>, Stjepan Šarić<sup>1</sup>, Imre Szenti<sup>3</sup>, Tina Skalar<sup>4</sup>, Matjaž Finšgar<sup>5</sup>, Mi Tian<sup>2</sup>, Ákos Kukovecz<sup>3</sup>, Zoltán Kónya<sup>3</sup>, András Sápi<sup>3</sup> <sup>1</sup>Department of Chemistry, Josip Juraj Strossmayer University of Osijek, Cara Hadrijana 8/A, HR–31000 Osijek, Croatia <sup>2</sup>Department of Engineering, Faculty of Environment, Science and Economy, University of Exeter, Penryn Campus, Cornwall TR10 9FE, United Kingdom <sup>3</sup>Department of Applied and Environmental Chemistry, University of Szeged, Rerrich Béla Sq. 1, H–6720 Szeged, Hungary <sup>4</sup>Faculty of Chemistry and Chemical Technology, University of Ljubljana, Večna pot 113, SI–1000 Ljubljana, Slovenia <sup>5</sup>Faculty of Chemistry and Chemical Engineering, University of Maribor, Smetanova street 17, SI–2000 Maribor. Slovenia

Herein, we investigate the potential of nanostructured high–entropy oxides (HEOs) for photocatalytic CO<sub>2</sub> hydrogenation, a process with significant implications for environmental sustainability and energy production. Several cerium–oxide–based rare–earth HEOs with fluorite structures were prepared for UV–light driven photocatalytic CO<sub>2</sub> hydrogenation towards valuable fuels and petrochemical precursors. The cationic composition profoundly influences the selectivity and activity of the HEOs, where the  $Ce_{0.2}Zr_{0.2}La_{0.2}Nd_{0.2}Sm_{0.2}O_{2-\delta}$  catalyst showed outstanding CO<sub>2</sub> activation (14.4 mol<sub>co</sub> kg<sub>cat</sub><sup>-1</sup> h<sup>-1</sup> and 1.27 mol<sub>CH3OH</sub> kg<sub>cat</sub><sup>-1</sup> h<sup>-1</sup>) and high methanol and CO selectivity (7.84 % CH<sub>3</sub>OH and 89.26 % CO) at ambient conditions with 4–times better performance in comparison to pristine CeO<sub>2</sub>. Systematic tests showed the effect of a high–entropy system compared to mid–entropy oxides. XPS, *in situ* DRIFTS as well as DFT calculation elucidate the synergistic impact of Ce, Zr, La, Nd, and Sm, resulting in an optimal Ce<sup>3+</sup>/Ce<sup>4+</sup> ratio. The observed formate–routed mechanism and a surface with high affinity to CO<sub>2</sub> reduction offer insights into the photocatalytic enhancement. While our findings lay a solid foundation, further research is needed to optimize these catalysts and expand their applications.

# State diagrams of systems based on iron oxide and REE as a basis for creating magnetic materials

Olga Chudinovych<sup>1,2</sup>, Olena Olifan<sup>1</sup> <sup>1</sup>Frantsevich Institute for Problems of Materials Science of the NAS of Ukraine, Omeliana Pritsaka str. 3, Kyiv-03142, Ukraine <sup>2</sup>National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Peremohy Av. 37, Kyiv-03056, Ukraine

Today, it is important to create new materials with high magnetic properties. Chemical compounds of iron oxide  $Fe_2O_3$  with oxides of rare earth metals  $Ln_2O_3$  have special magnetic (ferromagnetic) properties that combine high magnetization and semiconductor or dielectric properties, thanks to which they have been widely used as magnetic materials in radio engineering, radio electronics, computer technology, catalysis, gas separation fuel cells, magneto-optical devices. In recent years, rare-earth orthoferrites RFeO<sub>3</sub> have become the focus of research for the development of multiferroics. Some RFeO<sub>3</sub> orthoferrites can exhibit an unusual coexistence of ferroelectricity and weak ferromagnetism. The study of phase equilibria in systems based on REE oxides will provide an opportunity to form a theoretical basis for creating new materials, which allows for determining the optimal compositions of materials, technological parameters of their production, and conditions of operation.

Powders of  $Ln_2O_3$  (99.99 %) and  $Fe(NO_3)_3 \times 6H_2O$  were used as raw materials. The samples were prepared in steps of 1 and 5 mol.% from nitrate solutions with their subsequent evaporation and decomposition at 800 °C for 2 h. Powders were pressed at 10 MPa into pellets of 5 mm in diameter and 4 mm in height. Thermal treatments were carried out in the furnaces with heating elements based on MoSi<sub>2</sub> (1300 °C) in air.

The samples were subjected to X-ray powder diffraction using a DRON-3 diffractometer at room temperature (Cu-K $\alpha$  radiation). The microstructures of the samples were studied by scanning electron microscopy with a Superprobe-733 analyzer (JEOL, Japan) in back-scattered electrons (BSE) and secondary electrons (SE).

The phase diagram for the  $Ln_2O_3$ -Fe<sub>2</sub>O<sub>3</sub> systems has been developed. It was established that in the  $Ln_2O_3$ -Fe<sub>2</sub>O<sub>3</sub> systems there exist fields based on hexagonal (A) modification of  $Ln_2O_3$ , rhombic modification of Fe<sub>2</sub>O<sub>3</sub>, as well as perovskite-type ordered phase of orthorhombic symmetry  $LnFeO_3$  (R). Solubility limits are determined and concentration dependencies of periods also lattice parameters of the unit cell of phases formed in the systems are constructed.

# Graphene oxide-based nanocomposites on interdigital electrodes for sensing applications

<u>Željko Mravik</u><sup>1</sup>, Milica Pejčić<sup>2</sup>, Marija Grujičić<sup>2</sup>, Jelena Rmuš Mravik<sup>1</sup>, Predrag Stolić<sup>3</sup>, Sonja Jovanović<sup>2</sup>, Zoran Jovanović<sup>1</sup>

<sup>1</sup>Center of Excellence for Hydrogen and Renewable Energy (CONVINCE), Laboratory of Physics, Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia

<sup>2</sup>Laboratory of Physics, Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia <sup>3</sup>Technical faculty in Bor, University of Belgrade, Serbia, Bor

The expansion of urban areas, increased car usage, rising air traffic, and other developments of the twenty-first century significantly impact the climate, making the development of sensing materials with high sensitivity and selectivity to the environmental conditions an important task. Graphene oxide (GO) is a contemporary material that has attracted significant scientific interest due to its 2D nature, unique structure featuring alternating  $sp^2$  and oxidized  $sp^3$ regions, and easily modifiable surface chemistry. 2D nature of GO provides an opportunity for additional functionalization by incorporation of smaller molecules and particles onto the GO sheets. The modification of any of these properties influences the electrical properties, which can be monitored and directly correlated to environmental parameters. In order to investigate the application of GO-based nanocomposites for sensing application, thin layers of GO composite with 12-tungstophosphoric acid (WPA), cobalt-ferrite nanoparticles (CFO) and 3,4,9,10-perylene-tetracarboxylic acid-dianhydride were deposited onto the interdigital electrode by drop casting and dip coating method. The electric properties of pristine and modified sample (thermal and hydrothermal treatment) were investigated by impedance spectroscopy method in range from 10 Hz to 100 kHz. The results demonstrate that most of the materials exhibit good sensitivity to the change of environmental conditions. Specifically, thermally treated GO/WPA composites show a linear dependence of impedance values on temperature at low frequencies, while hydrothermally treated GO/CFO composites exhibit excellent sensitivity and good reversibility to even small moisture changes. These findings highlight the potential of GO-based nanocomposites for application in sensing devices.

*Acknowledgments*: This research was supported by the Science Fund of the Republic of Serbia, grant No. 6706, Low-dimensional nanomaterials for energy storage and sensing applications: Innovation through synergy of action – ASPIRE and by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia (contract No. 451-03-66/2024-03/200017).

# Synthesis of a hybrid core-shell nanoparticles for efficient photocatalysis under sunlight

Ivana Dinić<sup>1</sup>, Marina Vuković<sup>1</sup>, Bojan A. Marinković<sup>2</sup>, Paula Jardim<sup>3</sup>, Lidija Mančić<sup>1</sup> <sup>1</sup>Institute of Technical Science of SASA, Kneza Mihaila 35/4, Belgrade, Serbia <sup>2</sup>Department of Chemical and Materials Engineering, Pontifical Catholic University of Rio de Janeiro Rio de Janeiro, RJ, Brazil <sup>3</sup>Department of Metallurgical and Materials Engineering, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil

New up-converting hybrid core-shell nanoparticles of  $\alpha$ -NaYF<sub>4</sub>:Yb,Tm@TiO<sub>2</sub>-Acac, were synthesized by a two-step wet chemical route. Up-converting  $\alpha$ -NaYF<sub>4</sub>:Yb,Tm core, which converts near-infrared (NIR) to visible (VIS) light, was obtained through EDTA assisted hydrothermal process, while the shell of anatase TiO<sub>2</sub>-Acetylacetonate charge transfer complex (TiO<sub>2</sub>-Acac), which ensures absorption of VIS light, was formed via by sol-gel method. Tetracycline was used to investigate the photocatalytic efficiency of obtained materials under irradiation of a solar simulator. Because  ${}^{1}D_{2}\rightarrow {}^{3}F_{4}$  and  ${}^{1}G_{4}\rightarrow {}^{3}H_{6}$  emission of Tm<sup>3+</sup> match well with the absorption edge of TiO<sub>2</sub>-Acac, radiation-reabsorption and Förster resonance energy transfer (FRET) processes enhance the overall generation of reactive oxygen species and degradation of tetracycline. Using scavengers, p-benzoquinone (PBQ) and isopropyl alcohol (IPA), implicated that 'O<sup>2-</sup> ions are mainly responsible for tetracycline degradation. After 6 hours of photocatalysis, approximately 90 % of the tetracycline was successfully degraded under a solar simulator.

### Phonon Contribution in the Heat Conductivity of Some Typical Models of Crystalline Nanostructures

Jovan P. Šetrajčić<sup>1</sup>, Dušan I. Ilić<sup>2</sup> <sup>1</sup>Academy of Sciences and Arts of the Republic of Srpska, Banja Luka, Republic of Srpska, Bosnia and Herzegovina <sup>2</sup> University of Novi Sad, Faculty of Technical Sciences, Novi Sad, Vojvodina, Serbia

Using the adapted method of two-time temperature-dependent Green's functions with differential variables, we have recently completed the theory of calculating the thermodynamic properties of some characteristic crystalline nanostructures. Based on the found law of phonon dispersion, in this paper we determined the thermal conductivity coefficient of the superlattice using the definition of internal and free energy, and then compared their temperature dependence with the previously determined temperature behavior of the thermal conductivity of ultrathin films and, known - bulk crystal structures. For the observed nanostructures at low temperatures, the values of thermal conductivity coefficients are almost identical, but at the same time they are significantly lower than the same values for bulk samples of the same chemical and crystallographic structure. This result is useful for expanding knowledge about the mechanisms of the occurrence of specific conditions in high-temperature superconductors in which their significantly better properties are achieved.

### Influence of synthesis conditions of ZIF-67/polyaniline 5-sulfosalicylate composites on the properties and electrochemical behavior of their carbonization derivatives

Maja Ranković<sup>1</sup>, <u>Aleksandra Janošević Ležaić</u><sup>2</sup>, Marjetka Savić<sup>3</sup>, Nemanja Gavrilov<sup>1</sup>, Danica Bajuk-Bogdanović<sup>1</sup>, Igor Pašti<sup>1</sup>, Gordana Ćirić-Marjanović<sup>1</sup> <sup>1</sup>University of Belgrade-Faculty of Physical Chemistry, Studentski trg 12-16, 11158 Belgrade, Serbia <sup>2</sup>University of Belgrade-Faculty of Pharmacy, Belgrade, Vojvode Stepe 450, 11221 Belgrade, <sup>3</sup>Vinča Institute of Nuclear Science, University of Belgrade, National Institute of the Republic of Serbia, P.O. Box 522, 11001 Belarade. Serbia

Composites of carbons with metal/metal oxides have attracted significant interest due to their remarkable characteristics, including large surface area and a wide range of chemical functionalities, as materials for energy conversion and storage applications. Herein we explore the impact of a Co-containing metal-organic framework (MOF), ZIF-67, on the formation of self-assembled polyaniline (PANI) 5-sulfosalicylate nanorods/nanotubes (PANISSA). Synthesized ZIF-67/PANISSA composites are carbonized in an inert atmosphere. The materials are characterized by various techniques (SEM, FTIR, Raman, electrical conductivity measurements). The electrochemical performance of novel Co/N,O-doped carbon composites (C-(ZIF67/PANISSA)), synthesized by carbonization of ZIF-67 /PANI-SSA composites was studied. Composite formation was scrutinized for the time of addition of pre-formed ZIF-67 to the aniline polymerization medium using ammonium peroxydisulfate as oxidant, in the presence of 5-sulfosalicylic acid (SSA). SEM images showed that the addition time significantly influences the obtained ZIF67/PANISSA composites morphology, which can be tuned from dominant nanorods/nanotubes to granular morphology. The capacitance of the carbonization derivatives, C-(ZIF67/PANISSA) composites, was evaluated in alkaline and acidic environments with values reaching as high as 145 and 122 F/g respectively, at a low sweep rate of 5 mV/s. The properties and capacitance of C-(ZIF67/PANISSA) composites depended on the ZIF67/PANISSA precursors properties, affected by the time of ZIF-67 addition. The study suggests that in composite formation the addition time of MOF to the aniline polymerization reaction system can be crucial as it can significantly alter the polymerization process leading to different product morphology, conductivity and other properties, which can in turn influence the electrochemical behavior of composite materials derived from their carbonization.

#### Photocatalytic properties of Mo, W and Cu-doped bismuth vanadate

Marko Jelić<sup>1</sup>, Danica Bajuk-Bogdanović<sup>2</sup>, Igor Pašti<sup>2</sup>, Jelena Erčić<sup>1</sup>, Zoran Jovanović<sup>1</sup>, <u>Sonja Jovanović<sup>1</sup></u> <sup>1</sup>Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia

<sup>2</sup>Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia

One of the primary challenges in photocatalytic purification of dye-containing wastewater is development of efficient photocatalysts. Lately, bismuth vanadate (BiVO<sub>4</sub>, BVO) has attracted attention due to its visible light harvesting properties, band edge positions and low-cost synthesis method. Herein, we report physicochemical and photocatalytic properties of solvothermally synthesized 5 % Mo, W and Cu-doped BVO powders at 180 °C for 8 h. X-ray diffraction and Raman spectroscopy indicate that, depending on the type of dopant, material exists in monoclinic scheelite or tetragonal zircon phase. Monoclinic phase was formed in a case of pristine. Mo and W-doped BVO samples while tetragonal zircon phase was observed in case of Cu-doped sample. Scanning electron microscopy revealed that monoclinic scheelite BVO exhibits elongated assembly of cube-like particles, while tetragonal zircon BVO consistently shows particles of porous spherical shape. Optical properties were characterized with UV-Vis Diffuse Reflectance Spectroscopy and Photoluminescence (PL) spectroscopy. Pristine, Mo and W-doped samples showed band gap in the range 2.35 - 2.52 eV while Cu-doped samples showed band gap of 2.9 eV. PL results indicate that monoclinic samples possess better recombination features than tetragonal ones. The results revealed better photocatalytic degradation of methylene blue by BVO in monoclinic scheelite phase compared to tetragonal zircon phase. Also, it was found that the type of dopant (W, Mo) plays an important role in degradation efficiency of BVO in monoclinic scheelite phase.

*Acknowledgements:* This research was supported by the Science Fund of the Republic of Serbia, grant No. 6706, Low-dimensional nanomaterials for energy storage and sensing applications: Innovation through synergy of action – ASPIRE and by the Ministry of Science, Technological Development and Innovation (MoSTI) of the Republic of Serbia (Grant no. 451-03-66/2024-03/20017 and 451-03-66/2024-03/200146) and and bilateral project of Serbia - Slovenia scientific collaboration (Grant no. 337-00-110/2023-05/28).

#### P.S.II.D.4

# Tesla inspired quantum-holographic non-local epigenetic clue for improving integrative medicine & transpersonal psychology

Dejan Raković University of Belgrade, Faculty of Electrical Engineering, Belgrade, Serbia

Nikola Tesla is undoubtedly the greatest inventor in the history of electrical engineering, and what makes him especially fascinating was his unusual mental control of creative visions, with possibility of meditative eidetic control and increase of macroscopic quantum correlations with the quantum-holographic primal source of collective consciousness. These insights could also provide deeper understanding of our extended Hopfield-like macroscopic quantum-holographic / quantum gravitational (QHQG) framework for non-local psychosomatics, based on decrease of quantum entropy & macroscopic quantum correlations of acupuncture system / individual consciousness & collective consciousness, which may help in developing future epigenetic strategies for integrative medicine & transpersonal psychology. In wider context, Tesla's whole research and life could also provide an inspiration for reconsideration of global educational / political goals – with orientation towards holistic gentle actions for solutions of global risk society.

#### P.S.II.D.5

## Co-ZSM5 and CoNi-ZSM5 zeolites for ORR in alkaline media

Jadranka Milikić<sup>1</sup>, Srna Stojanović<sup>1</sup>, Katarina Rondović<sup>1</sup>, Ljiljana Damjanović-Vasilić<sup>1</sup>, Vladislav Rac<sup>2</sup>, Kristina Radinović<sup>1</sup>, Biljana Šljukić<sup>1,3</sup> <sup>1</sup>University of Belgrade, Faculty of Physical Chemistry, Studentski trg 12-16, 11158 Belgrade, Serbia <sup>2</sup>University of Belgrade, Faculty of Agriculture, Nemanjina 6, 11080 Belgrade, Serbia <sup>3</sup>Center of Physics and Engineering of Advanced Materials, Laboratory for Physics of Materials and Emerging Technologies, Chemical Engineering Department, Instituto Superior Técnico, Universidade de Lisboa, 1049-001 Lisbon, Portugal

Oxygen reduction reaction (ORR) presents a cathode reaction in proton exchange membrane fuel cells (PEMFC) and metal-air batteries (MABs). It is well known that noble platinum (Pt) and platinum-based electrocatalysts present the best ORR electrocatalysts. On the other hand, these electrocatalysts have high prices and low ORR stability, which limits their practical application. In this paper, two cobalt ZSM-5 zeolites (Co-ZSM5 and CoNi-ZSM5) are synthesized by an ion exchange procedure of synthetic zeolite ZSM-5 and examined for ORR in alkaline media. Morphology, structure, and elemental analysis of these electrocatalysts were investigated by X-ray powder diffraction, Fourier transform infrared spectroscopy, and scanning electron microscopy with energy dispersive spectroscopy. The electrochemical investigation was done by cyclic voltammetry (CV) and linear sweep voltammetry with a rotating disk electrode (LSV RDE) in 1 M KOH solution. Both Co-ZSM5 and CoNi-ZSM5 electrocatalysts showed high ORR activity. Namely, CoNi-ZSM5 gave an even two times higher ORR current density (-1.6 mA cm<sup>-2</sup>) than Co-ZSM5 (-0.7 mA cm<sup>-2</sup>) at 0.4 V vs. RHE and a rotation rate of 1200 rpm. Onset potential (Eonset) of 0.77 and 0.78 V vs. RHE was obtained for Co-ZSM5 and CoNi-ZSM5, respectively, at a current density of -0.1 mA cm<sup>-2</sup>. These obtained results are in agreement with similar literature reports [1].

#### **References:**

1. Milikić, J.; Stojanović, S.; Damjanović-Vasilić, L.; Vasilić, R.; Šljukić, B. Efficient bifunctional cerium-zeolite electrocatalysts for oxygen evolution and oxygen reduction reactions in alkaline media. *Synth. Met.* **2023**, *292*, 117231. https://doi.org/10.1016/j.synthmet.2022.117231.

#### P.S.II.D.6

#### Incorporation of natural pyrophyllite into wood polymer composites

<u>Srđan Perišić</u><sup>1</sup>, Anđela Radisavljević<sup>1</sup>, Aleksandar Grujić<sup>2</sup>, Jasna Stajić-Trošić<sup>2</sup>, Vesna Radojević<sup>3</sup> <sup>1</sup>University of Belgrade, Innovation Centre of the Faculty of Technology and Metallurgy, Belgrade, Serbia <sup>2</sup>University of Belgrade, Institute of Chemistry, Technology and Metallurgy, National Institute of the Republic of Serbia, Belgrade, Serbia

<sup>3</sup>University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia

Wood polymer composites (WPCs) with incorporated biodegradable natural fibers offer benefits such as low density, high strength, excellent impact properties, eco-friendliness, and cost-effectiveness. They are widely used in automotive, civil engineering, and interior/exterior design industries, replacing traditional polymer composites. In this study, the influence of hybridization of the matrix and the addition of natural pyrophyllite on the moisture resistance and mechanical properties of composites were examined.

Three series of composites were blended using a high-speed mixer: Composite 1 - C1 (60 wt.% high-density polyethylene (HDPE), 36 wt.% oak wood flour from sawmill (wood), 4 wt.% Fusabond Du Pont WPC-576D (FB)); Composite 2 - C2 (60 wt.% HDPE, 26 wt.% wood, 4 wt.% FB, 10 wt.% Pyrophyllite powder (PHY)); and Composite 3 - C3 (30 w.t% HDPE, 26 wt.% wood, 4 wt.% FB, 10 wt.% PHY, 30 wt.% waste HDPE (WP)). The blended mixture was extruded through a screw extruder to form composite bars and granulated with a universal cutting machine. The WPC composition was shaped using a steel mold under isostatic pressure.

The results of the moisture absorption test indicate that the choice of raw materials and the processing conditions of the composite affect the moisture absorption resistance of the final product. The addition of pyrophyllite powder reduced water absorption and swelling. Morphological analysis showed water absorption alters composite microstructure due to its hydrophilic nature. Thermal analysis established that C2 exhibits the highest melting temperature ( $T_m$ ) and glass transition temperature ( $T_g$ ) values. Dynamic mechanical analysis demonstrated that C2 had the highest storage modulus (E) at lower strain levels, while C3 showed higher E at higher strain levels. C3 exhibited the highest tan  $\delta$  value, indicating superior mechanical damping and viscoelastic properties.

The study's findings indicate that incorporating PHY particles significantly improves the weather resistance, thermal stability, and mechanical properties of WPCs.

### Novel biocomposites based on activated charcoal and probiotics ProHealingAC project

<u>Vesna Lazić</u><sup>1</sup>, Tanja Krunić<sup>2</sup>, Sonja Mojsilović<sup>3</sup>, Miloš Đuknić<sup>4</sup>, Andrea Osmokrović<sup>5</sup> <sup>1</sup>University of Belgrade, Faculty of Agriculture, Belgrade, Serbia <sup>2</sup>University of Belgrade, Innovation Center, Faculty of Technology and Metallurgy, Belgrade, Serbia <sup>3</sup>University of Belgrade, Institute for Medical Research, Belgrade, Serbia <sup>4</sup>University of Belgrade, Faculty of Medicine (School of Medicine), Belgrade, Serbia <sup>5</sup>University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia

Antibiotic resistance is one of the most important public health threats that humanity is facing today [1]. The overuse and misuse of antibiotics have led to the global clinical problem concerning the treatment of resistant pathogens. Development of conventional drugs is going slowly, so new innovative approaches are urgently needed in developing novel therapies. The two-year ProHealingAC project, funded by the Science Fund of the Republic of Serbia, strives to develop a novel strategy for prevention and local treatment of wound infections. Precisely, a multidisciplinary ProHealingAC team intends to develop biocomposites (BCs) based on activated charcoal (AC) and probiotic microorganisms with their sustained local release in the wound area by combining the principles of engineering and life sciences. Previously, it has been shown that activated charcoal (AC) in conjunction with different active agents has an efficient antimicrobial activity [2,3]. In addition, focus has been put to the influence of glucose level (normo- and hyperglycemia) in the microenvironment of the wound. Developed BCs will be comprehensively characterized in *in vitro* and *in vivo* conditions. Precisely, BCs will be investigated regarding probiotic release profile, antimicrobial and antibiofilm activity as well as modulation of macrophage, fibroblast and keratinocyte activity. The best BC, based on the obtained results, will be examined in the wound model in diabetic and non-diabetic animals. In addition, efficient dissemination and communication of the results will help raise public awareness of the importance of the rational use of antibiotics in both human and veterinary medicine as well.

*Acknowledgement*: This research was supported by the Science Fund of the Republic of Serbia, Grant No 9802, Activated Charcoal as a Carrier of Probiotics: A New Approach for Pathogen Elimination in Wounds - ProHealingAC.

### **References:**

- 1. Available online: <u>https://www.who.int/news-room/fact-sheets/detail/antibiotic-resistance</u>
- Osmokrovic, A.; Jancic, I.; Vunduk, J.; Petrovic, P.; Milenkovic, M.; Obradovic, B. Achieving high antimicrobial activity: composite alginate hydrogel beads releasing activated charcoal with an immobilized active agent. *Carb. Pol.* 2018, *196*, 279–288. https://doi.org/10.1016/j.carbpol.2018.05.045
- 3. Osmokrovic, A.; Jancic, I.; Jankovic-Castvan, I.; Petrovic, P.; Obradovic, B. Novel composite zincalginate hydrogels with activated charcoal aimed for potential applications in multifunctional primary wound dressings. *Hem. Ind.* **2019**, *73*, 37–46.

# Study of copper-doped hydroxyapatite and copper-doped silicate-substituted nanohydroxyapatite as antibacterial and antifungal materials

<u>Nataliia Dmytrivna Pinchuk</u><sup>1,2</sup>, Agata Piecuch<sup>3</sup>, Sara Targońska<sup>2,4</sup>, Paulina Sobierajska<sup>2</sup>, Katarzyna Szyszka<sup>2</sup>, Oleksii Bezkrovnyi<sup>2</sup>, Rafał Ogórek<sup>3</sup>, Rafal Jakub Wiglusz<sup>2,5</sup>

<sup>1</sup>Department of Functional Materials for Medical Application, Frantsevich Institute for Problems of Materials Science of the NAS of Ukraine, Pritsaka, 3, Kyiv, 03142, Ukraine

<sup>2</sup>Division of Biomedical Physicochemistry, Institute of Low Temperature and Structure Research Polish Academy of Sciences, Okolna 2, 50-422, Wrocław, Poland

<sup>3</sup>Department of Mycology and Genetics, Institute of Genetics and Microbiology, University of Wroclaw, Przybyszewskiego 63/77, 51-148 Wroclaw, Poland

<sup>4</sup>Department of Molecular Sciences, Swedish University of Agricultural Sciences, Box 7015, 75007 Uppsala, Sweden

<sup>5</sup>Department of Organic Chemistry, Bioorganic Chemistry and Biotechnology, Silesian University of Technology, Krzywoustego 4, 44-100 Gliwice, Poland

Hydroxyapatite is a widely demanded material known for its biocompatible and bioactive properties. A chemical element such as copper can become a promising additive to hydroxyapatite to improve its bioactive properties, namely antifungal and antibacterial properties.

In this work, nanopowders of hydroxyapatite doped with copper and silicate-substituted nanohydroxyapatite doped with copper ions were obtained by the microwave-assisted hydrothermal method with next sintering at the temperature of 450 °C. The doping of the copper ions in the samples was 0.1, 0.5, and 1 mol.% from the calcium ions. Crystal structure, chemical composition, and morphology of prepared nanopowders were investigated by using X-ray powder diffraction analysis, EDX analysis, Fourier transform infrared spectroscopy, and transmission electron microscopy. The effect of cationic substitution with copper in these different types of hydroxyapatite on their structure, morphology, and properties, especially antibacterial and antifungal activity, was investigated.

Hydroxyapatite and silicate-substituted hydroxyapatite both doped with copper ions showed antibacterial activity in comparison to pure hydroxyapatite against gram-positive bacteria strains in contradistinction to gram-negative bacteria. These materials also demonstrated antifungal activity, namely inhibition of fungal growth against reference strains *C. albicans*, *C. kruzei*, and *C. tropicalis*.

### Antibacterial electrospun poly(ε-caprolactone) nanofiber mats loaded with cefazolin and meropenem for wound healing

<u>Anđela Radisavljević</u><sup>1</sup>, Jasmina Stojkovska<sup>2</sup>, Ivan Jančić<sup>3</sup>, Dragana Božić<sup>3</sup>, Srđan Perišić<sup>1</sup>, Dušica Stojanović<sup>2</sup>, Petar Uskoković<sup>2</sup>

<sup>1</sup>University of Belgrade, Innovation Centre of the Faculty of Technology and Metallurgy, Belgrade, Karnegijeva 4, 11120 Belgrade, Serbia

<sup>2</sup>University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11120 Belgrade, Serbia <sup>3</sup>University of Belgrade, Faculty of Pharmacy, Vojvode Stepe 450, 11221 Belgrade, Serbia

Nanofiber wound dressings represent a promising approach to wound care, offering an adaptable platform for promoting faster and more effective wound healing. The goal of this research was the development of  $poly(\epsilon$ -caprolactone) (PCL) nanofiber mats with incorporated antibiotics cefazolin (CEF) and meropenem (MER) for wound healing treatments.

Nanofiber mats based on PCL (8 wt.% PCL prepared in 2,2,2-trifluoroethanol (TFE)) with cefazolin or meropenem (10 % of the polymer's weight) were produced using the blend electrospinning method. For comparison, PCL nanofibers without antibiotics were prepared by dissolving PCL pellets in TFE. The electrospinning parameters were a flow rate of 2.7 ml/h for PCL/CEF and 3 ml/h for neat PCL and PCL/MER solutions. The distance from the collector was 10 cm, and the voltage was 29 kV for all solutions.

In the processed samples, cefazolin and meropenem maintained their biological activity and did not react with the PCL. The drug release profiles showed that the PCL/CEF released about 60 % of the drug, while the PCL/MER released about 40 % after 48 hours of incubation in Mueller-Hinton broth. Both PCL/CEF and PCL/MER nanofiber mats showed similar growth delays of Gram-positive clinical strains (*S. aureus* and *S. epidermidis*) compared to neat PCL. However, PCL/MER nanofiber mats efficiently inhibited the growth of Gram-negative clinical strains (*E. coli*, Klebsiella, *Enterobacter spp.*, and *Acinetobacter spp.*). The effective antibacterial action of PCL/MER nanofiber mats could minimize infection-related inflammation, reducing the risk of complications like delayed healing, sepsis, and chronic wound formation.

The overall results of this study have shown that novel PCL nanofiber mats could be used as a relevant drug scaffold, keeping the wound infection-free and promoting faster and more effective tissue repair.

### 3D Printable Polyhydroxyalkanoate Hydrogels as Potential Scaffolds for Cartilage Replacement

Zuzana Kadlecová<sup>1</sup>, Nicole Černeková<sup>2</sup>, Adriána Kovalčík<sup>2</sup>, Lucy Vojtová<sup>1</sup> <sup>1</sup>Central European Research Institute, Brno University of Technology, Czechia <sup>2</sup>Faculty of Chemistry, Brno University of Technology, Czechia

Osteoarthritis affects approximately 10-12 % of the global population and causes significant pain and impaired joint function [1]. Despite this, conventional therapy, such as total joint arthroplasty, imposes considerable economic and patient-related burdens. Our study investigated the potential of polyhydroxyalkanoate (PHA) hydrogels as cartilage replacement scaffolds by employing low-temperature three-dimensional printing and leveraging PHA's biocompatibility, biodegradability, and mechanical properties.

Polyhydroxyalkanoates, specifically poly(3-hydroxybutyrate) (P3HB) and its copolymers with poly(4-hydroxybutyrate) (P4HB), are promising materials for cartilage tissue engineering because of their desirable mechanical properties similar to those of cartilage, such as Young's modulus and viscoelastic modulus [2]. However, their hydrophobic nature hinders hydrogel formation. To overcome this limitation, a solvent-exchange method using water-miscible solvents, including dimethyl sulfoxide (DMSO) and acetic acid, was adopted to facilitate the transition from organogels to hydrogels. The hydrogels were further 3D printed using direct ink writing (DIW), a low-temperature 3D printing method, to preserve the bioactivity of the encapsulated cells and growth factors.

Pure P3HB and P4HB and their blends with agarose were prepared. The structural and mechanical properties of each formulation were evaluated, with a focus on characterisation using FTIR and XRD. The transition temperatures of the blends were determined using TGA. The successful preparation of PHA-based hydrogels intended for 3D printing was supported by the injectability and rheological properties results.

Acknowledgment: This work was supported by the Internal Grants of BUT (Specific Research) Reg. No. BD162404002 and also by the project MeBioSys funded as project No. CZ.02.01.01/00/22\_008/0004634 by Programme Johannes Amos Comenius, call Excellent Research. CzechNanoLab project LM2018110, funded by MEYS CR, is gratefully acknowledged for financial support of the measurements at the CEITEC Nano Research Infrastructure.

1. HU, Z., et al., 2019. Clin Med Chin, 35, 566-71.

2. Yang, F., et al., 2017. ACS biomaterials science & engineering, 3 (5), 863-869.

# Feed additives based on polyvalent nanodisperse iron oxides, obtained by the electroerosion dispersion method, for feeding broiler chickens

Tetiana Prikhna<sup>1</sup>, Mykola Monastyrov<sup>1</sup>, Olena Prysiazhna<sup>1</sup>, <u>Iryna Galstian</u><sup>2</sup>, Fernand Marquis<sup>3</sup>, Vasyl Kovalenko<sup>4</sup>, Mykola Novohatskyi<sup>5</sup>, Branko Matović<sup>6</sup>, Ivana Cvijović-Alagić<sup>6</sup>, Jerzy Madej<sup>7</sup>

<sup>1</sup>V. Bakul Institute for Superhard Materials of the National Academy of Sciences of Ukraine, Kiev, Ukraine

<sup>2</sup>G. V. Kurdyumov Institute for Metal Physics of the N.A.S. of Ukraine, 36 Academician Vernadsky Boulevard, UA-03142 Kviv, Ukraine

<sup>3</sup>San Diego State University, San Diego, United States

<sup>4</sup>National University of Life and Environmental Science of Ukraine

<sup>5</sup>Leonid Pogorilyy Ukrainian Scientific Research Institute of Forecasting and Testing of Machinery and

Technologies for Agricultural Production of the Ministry of Economy of Ukraine, Doslidnytske,

Vasylkivskyi district, Kyiv region, Ukraine

<sup>6</sup>MSL, Vinča Institute of Nuclear Sciences, Belgrade University, Belgrade, 11001 Serbia <sup>7</sup>LLC "New Heating Technology", Bytom, Poland

Nanodispersed iron oxides, obtained using the electroerosion dispersion (EED) technology, were used to produce feed additive Nano-Fe+<sup>TM</sup>, developed by M. Monastyrov. The efficiency of nano-Fe+<sup>TM</sup> (feed premixes for growing broiler chickens) based on nano-oxides of iron powder dissolved in glycerol or polyethyleneglycol was studied. The powders obtained by EED-method showed excellent functional properties. The method of increasing the productivity of agricultural animals and birds is to introduce iron nanopowder into the feeding ration by spraying feed with a suspension of iron nanopowder with a particle size of 20-30 nm in doses of 0.08-0.1 mg/kg of live weight per day. Additive nanomagnetite premix can be given both in dry form and in the form of spraying with a prepared suspension. At the poultry factory, the suspension is diluted in water at the rate of 1 ml / 1 l. The solution of the drug is sprayed on poultry feed before feeding at the rate of 10 l/1 ton of feed. The following results were obtained (in terms of qualitative indicators): increase in chicken body weight by 5 to 17 %; acceleration of growth rates of broilers by 10 to 20 %; increase in the protection of birds by 10 to 20 %; increase in the protection of birds by 10 to 20 %; increase in egg production of laying hens by 10 to 15 %; reducing the effects of stress from vaccination, regrouping, etc.

# SrTiO<sub>3</sub>-based nanoparticles in dental poly(methyl methacrylate): mechanical and thermal properties

Houda Taher Elhmali<sup>1</sup>, <u>Ivana Stajčić</u><sup>2</sup>, Miloš Petrović<sup>1</sup>, Aleksandar Stajčić<sup>3</sup>, Marija Jovanović<sup>1</sup>, Dušica B. Stojanović<sup>1</sup>, Petar Uskoković<sup>1</sup>, Vesna Radojević<sup>1</sup> <sup>1</sup>Faculty of Technology and Metallurgy, University of Belgrade, 11000 Belgrade, Serbia <sup>2</sup>Department of Physical Chemistry, "Vinča" Institute of Nuclear Sciences-National Institute of the Republic of Serbia, University of Belgrade, 11000 Belgrade, Serbia <sup>3</sup>Center for Microelectronic Technologies, Institute of Chemistry, Technology and Metallurgy-National Institute of the Republic of Serbia, University of Belgrade, 11000 Belgrade, Serbia

Poly(methyl methacrylate) (PMMA) for dental application offers advantages such as ease of fabrication, cost-effectiveness, and favorable physical and mechanical properties. However, these characteristics alone do not provide sufficient impact strength and hardness. As a result, pure PMMA is less suitable for dental applications. This research aimed to enhance the impact resistance and hardness of PMMA by incorporating hybrid nanoparticles based on SrTiO<sub>3</sub> (STO). Field emission scanning microscopy was used for the identification of agglomerates in the composites, as well as for the determination of toughening mechanisms at the fracture surface. Various toughening mechanisms were observed, with crack pinning being dominant. Differential scanning calorimetry was conducted to study the influence of nanoparticles on the glass transition temperature ( $T_g$ ) of PMMA. It was established that there was no significant influence on  $T_g$ . Mechanical property investigations revealed that the STO-based hybrid reinforcements significantly improved microhardness and total absorbed impact energy. The results of this study highlight the reinforcing potential of hybrid nanoparticles, suggesting that their application does not have to be limited to PMMA.

## Electroconductive electrospun PCL-MXene scaffolds for effective cardiac tissue regeneration

<u>Oleksiy Gogotsi</u><sup>1</sup>, Kateryna Diedkova<sup>2,3</sup>, Yevheniia Husak<sup>2,4</sup>, Wojciech Simka<sup>4</sup>, Viktoriia Korniienko<sup>2,3</sup>, Bojan Petrović<sup>5</sup>, Anton Roshchupkin<sup>2</sup>, Agnieszka Stolarczyk<sup>4</sup>, Natalia Waloszczyk<sup>5</sup>, Ilya Yanko<sup>2</sup>, Kaspars Jekabsons<sup>3</sup>, Maria Čaplovičová<sup>6</sup>, Alexander D. Pogrebnjak<sup>2,6</sup>, Veronika Zahorodna<sup>1</sup>, Serhii Dukhnovskiy<sup>1</sup>, Iryna Roslyk<sup>1</sup>, Ivan Baginskiy<sup>1,2</sup>, Marko Radović<sup>5</sup>, Sanja Kojić<sup>5</sup>, Una Riekstina<sup>3</sup>, Maksym Pogorielov<sup>2,3</sup> <sup>1</sup>Materials Research Centre, Kyiv, Ukraine <sup>2</sup>Sumy State University, Sumy, Ukraina <sup>3</sup>University of Latvia, Riga, Latvia <sup>4</sup>Silesian University of Technology, Gliwice, Poland <sup>5</sup>University of Novi Sad, Serbia <sup>6</sup>Slovak University of Technology in Bratislava, Slovakia

Our research is focused on development of novel patches for cardiac tissue regeneration. Integration of MXenes into electrospun polycaprolactone (PCL) membranes was studied in order to harness the unique properties of  $Ti_3C_2$  MXenes for creation of conductive, biocompatible, and mechanically robust scaffolds that promote cell adhesion, proliferation, and functional maturation. We demonstrate a new method for depositing  $Ti_3C_2T_x$  MXenes onto hydrophobic electrospun PCL membranes using oxygen plasma treatment. This innovative approach has a positive effect on fiber size and increasing porous structure, reducing the contact angle of the PCL membrane and provides deep impregnation of MXene into the material. The resulted PCL-MXene composite membrane is non-toxic, possess biomedical structural properties and electrical conductivity required for cardiac tissue regeneration, with no significant differences observed between the various numbers of MXene depositions. Incorporation of MXenes into biodegradable PCL membranes is very promising in conferring electroconductivity and enhancing cellular response in tissue-engineered cardiac patches. These novel cardiac patches with MXene coating have a big prospectives for real application

providing mechanical support to the damaged heart tissue and enabling electrical signal transmission, by mimicking the crucial electroconductivity required for normal cardiac function. After a detailed investigation of scaffold-to-cell interplay, including electrical stimulation, this technology has the potential for clinical application not only for cardiac regeneration, but also as neural and muscular tissue substitutes.

Acknowledgement: Supported by European Commission under HORIZON-Europe projects #101131147 "ESCULAPE", #101086184 "MX-MAP".

# Multi-ion-doped mesoporous bioactive glass particles as fillers in 3D printed biocomposite scaffolds

<u>Tamara Matić</u><sup>1</sup>, Teodora Jakovljević<sup>1</sup>, Vukašin Ugrinović<sup>2</sup>, Miloš Papić<sup>3</sup>, Đorđe Janaćković<sup>1</sup>, Rada Petrović<sup>1</sup>, Biljana Ljujić<sup>3</sup>, Đorđe Veljović<sup>1</sup> <sup>1</sup>University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia <sup>2</sup>Innovation Center of the Faculty of Technology and Metallurgy Ltd, Belgrade Serbia <sup>3</sup>University of Kragujevac, Faculty of Medical Sciences, Kragujevac, Serbia

Mesoporous bioactive glass particles (MBGs) doped with therapeutic ions present multifunctional particles for various biomedical applications owing to their great biocompatibility, biodegradability, bioactivity, and ability to simultaneously deliver therapeutic ions and drugs locally. The multi-ion doping approach allows tailoring of biological properties such as osteoinductive, angiogenic, and antimicrobial by incorporating angiogenic ions such as Cu and Mg, osteogenic ions like Mg and Sr, and antimicrobial ions like Cu and Zn. However, the amount of dopants must be controlled to avoid the cytotoxic effects of Cu and Zn ions. The aim of this study was to optimize synthesis parameters and cation content to obtain biocompatible multi-ion-doped MBGs and to fabricate 3D-printed biocomposite scaffolds based on poly(methacrylic acid), poly(ethylene glycol) diacrylate, gelatin, and multi-ion-doped MBGs.

A modified microemulsion-assisted sol-gel synthesis technique was used to obtain multi-iondoped MBGs, while a mask-stereolithography 3D printing method was employed to obtain scaffolds. The morphology and amorphous nature of MBGs were analyzed by FESEM and XRD analysis, while an MTT assay was performed on mouse bone marrow-derived stem cells (mBMSCs) to assess *in vitro* biocompatibility. The printability, swelling degree, and microstructure of 3D-printed scaffolds were also investigated.

The results indicate that the developed multi-ion-doped MBGs were completely biocompatible with mBMSCs and present promising particulate fillers for application in 3D-printed biocomposite scaffolds.

Acknowledgements: This research was funded by the Science Fund of Republic of Serbia #GRANT No.7470, Novel hybrid biomimetic macroporous composites with tuned biodegradability, improved osteointegration and anticancer properties for bone tissue regeneration – HyBioComBone and by Ministry of Science, Technological Development and Innovations, Republic of Serbia (No. 451-03-65/2024-03/200135, 451-03-66/2024-03/200287)

### P.S.III.A.8

# Sustainable synthesis of Ni(II) complex with 3,5-pyrazoledicarboxylic acid as ligand via mechanochemistry

<u>Nina Jovović</u>, Željko Jaćimović, Milica Kosović Perutović University of Montenegro, Faculty of Metallurgy and Technology, Cetinjski put bb, 81000 Podgorica, Montenegro

Mechanochemical syntheses are becoming more intensely studied in coordination chemistry because it can support reactions between solids quickly and quantitatively, with either no added solvent or only nominal amounts. Pyrazoles are five-membered heterocyclic organic compounds with a privileged structure, easily coordinated with transition metals, exhibiting a diverse range of agricultural and pharmaceutical activities.

The synthesis of 3,5-pyrazoledicarboxylic acid as a ligand with Ni(II) ions was performed using direct mixing and grinding methods in a zirconium ball mill jar. Syntheses were carried out with varying milling times. Both the direct product and the product obtained after the work-up were examined. The work-up involved adding ice into the jar and ball-milling the mixture. The solid synthesized complexes were characterized by elemental analysis, IR spectroscopy, and UV-Vis spectroscopy. The results reveal that the all obtained metal complexes are pure, single-component, and that the coordination of the metal with the ligand occurs via nitrogen and oxygen atoms after just 3 minutes of mixing.

A special contribution of this research is the development of simple synthesis method which, in a very short time, gives desired product without the use of solvents and additional refining.



#### 25<sup>th</sup> YUCOMAT 2024 & XIII WRTCS Herceg Novi, September 2 - 6, 2024

### P.S.III.A.9

### Solidification curves of Al-Cu-Mg alloys

<u>Biljana Zlatičanin</u><sup>1</sup>, Branislav Radonjić <sup>1</sup>Faculty of Metallurgy and Technology, Cetinjski put bb, 81000 Podgorica, Montenegro

Aluminum-copper-magnesium based alloys are the strongest casting alloys of aluminum. The copper content in these alloys varies between 4 and 10 % by weight, with most alloys containing around 5%. Many techniques are available to investigate the solidification of metals and alloys. Some of them were standardized such as DTA and DSC. Although these techniques are very accurate and well documented, they are inadequate for the industry to investigating the solidification of metals and alloys. The other way for investigating the solidification of metals and alloys is the cooling curve analysis method. This technique is based on the recording and analysis of temperature versus time data collected during the solidification of the sample. The derivative of the cooling curve improves the sensitivity of the measurements and allows better precision in determining the exact points of primary and eutectic solidification events. In this paper, solidification curves of Al-Cu-Mg alloys are experimentally determined. Also, solidification curves are obtained by calculation with the available JMatPro model. JMatPro's model has been developed for the calculation of various thermo-physical and physical properties with the aim of providing thermo-physical and physical properties for various types of multi-component-alloys during solidification. The subsequent comparison of the calculated and the gathered experimental results has shown that the experimental data support the results of the calculations guite well.

#### P.S.III.A.10

#### Double hot dip ZnAl coatings on reinforcement steel

<u>Anżelina Marek</u><sup>1</sup>, Veronika Steinerová<sup>2,3</sup>, Petr Pokorný<sup>2</sup>, Henryk Kania<sup>1</sup> <sup>1</sup>Silesian University of Technology, Faculty of Materials Engineering, Gliwice, Poland <sup>2</sup>Czech Technical University, Faculty of Architecture, Czech Republic <sup>3</sup>Czech Technical University, Klokner Institute, Prague, Czech Republic

This paper describes the microstructure (SEM) and corrosion behavior of Zn-5Al coatings obtained by double dipping on reinforcing steel. Based on micro-area chemical composition tests (EDS) and phase composition tests (XRD), the structural properties of the coating and corrosion products formed on the external surface after exposure to neutral salt mist (NSS) (EN ISO 9227) were identified. The growth kinetics of the Zn-5Al coating were used with complex parameters of the double hot dipping process. In the Fe-Al intermetallic layer, the occurrence of Fe(Al,Zn)<sub>3</sub> intermetallic phases was identified. It was found that the growth kinetics of Zn-5Al coatings and the thickness of the Fe(Al,Zn)<sub>3</sub> diffusion layer correlate with the thickness of the intermetallic Fe-Zn diffusion zinc coatings. NSS test main corrosion resistance Zn-5Al coatings with conventional hot-dip galvanizing coating. The increase in corrosion growth is the practical creation of protection of corrosion products: simonkolleite - Zn<sub>5</sub>(OH)<sub>8</sub>Cl<sub>2</sub>·H<sub>2</sub>O, but layered double hydroxides (LDH) contained on divalent cations Zn<sup>2+</sup>, trivalent cations Al<sup>3+</sup> and Cl<sup>-</sup> anions may also be formed locally.

### P.S.III.A.11

## Cost-efficient method for obtaining magnetic materials by processing iron-containing liquid waste

<u>Gennadii Kochetov</u>, Dmytro Samchenko, Oles Lastivka *Kyiv National University of Construction and Architecture, Ukraine* 

The known methods for production of magnetic materials are characterized by significant energy and resource consumption. The hydrophase ferritization is a promising cost-efficient method of synthesis, as it allows to obtain magnetic materials by processing of iron-containing industrial waste. Metallurgical enterprises generate a massive amount of toxic exhausted highconcentration etching solutions. Application of the ferritization process to recycle exhausted etching solutions allows to obtain marketable products from toxic industrial waste and at the same time can help to prevent environmental pollution. It enables a cost-efficient use of water at an industrial plant.

The aim of the study is to analyze qualitative and quantitative composition of the formed ferrite sediments and grain size of iron-containing particles. The various study parameters of ferritization were: initial pH values of the solutions, initial concentrations of total iron ions and duration of the aeration treatment of the reaction mixture. Thermal, as well as alternating magnetic field activations were used to initiate the ferritization process. The XRD showed that the formed sediments contained phases of  $\gamma$ -FeOOH,  $\delta$ -FeOOH, Fe<sub>3</sub>O<sub>4</sub>, and  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub>. Granulometry analysis showed that these sediments were highly dispersed and heterogeneous. Chemically stable phases of magnetite were obtained in the composition of sediments, with an initial concentration of iron in the reaction mixture of 16.6  $g/dm^3$ , pH of 11.5 and the process duration of 15 min. The study results demonstrated feasibility of further possible use of such sediments with a high magnetite content for production of materials with ferromagnetic and sorption properties. Thus, introduction of 15 % by mass, either of wastewater treatment sediments or spent polyvalent ferrum oxide sorbent in the composition of the protective powder coatings leads to improvement of the main mechanical properties of the coatings. And, moreover, obtained coatings increase shielding of electromagnetic radiation in the megahertz range by 4 times compared to standard ones.

#### Full cell sodium storage performance of biomass-derived non-graphitizable carbon

Jana Mišurović<sup>1</sup>, Aleksandra Gezović Miljanić<sup>1</sup>, Alen Vižintin<sup>2</sup>, Veselinka Grudić<sup>1</sup>, Robert Dominko<sup>2</sup>, Milica Vujković<sup>3,4</sup>

<sup>1</sup>University of Montenegro – Faculty of Metallurgy and Technology, Cetinjski put bb, 81000 Podgorica, Montenegro

<sup>2</sup>National Institute of Chemistry, Ljubljana 1000, Slovenia

<sup>3</sup>University of Belgrade – Faculty of Physical Chemistry, Studentski trg 12-16, 11158 Belgrade, Serbia <sup>4</sup>Center for Interdisciplinary and Multidisciplinary Studies, University of Montenegro, Podgorica. Montenegro

As the world is constantly developing, the demand for electricity is growing at an unprecedented rate. Future energy strategies are relying on still challenging, fluctuating renewable energy sources. Energy storage and conversion systems rise as crucial part of the consistent and efficient energy market.

To contribute to implementing sustainable and affordable energy storage devices into the renewable energy infrastructure, we have developed high-quality carbon anode (HC) for Na-ion batteries using abundant biowaste – vine shoots. Our anode, previously tested in half cell configuration vs. Na metal in NaPF<sub>6</sub>/EC+DMC+FEC electrolyte, exhibits low voltage, excellent cyclic stability and high specific capacity of  $\approx$ 270 mAh g<sup>-1</sup> at 37.2 mA g<sup>-1</sup> and  $\approx$ 253 mAh g<sup>-1</sup> at 372 mA g<sup>-1</sup>. Here we explore its full cell potential by pairing it with the commercial NVPF [Na<sub>3</sub>V<sub>2</sub>(PO<sub>4</sub>)<sub>2</sub>F<sub>3</sub>] cathode in a HC//NaPF<sub>6</sub>/EC+DMC+FEC//NVFP/C cell. This combination delivered high operating voltage of  $\approx$ 4 V with a reversible capacity of  $\approx$ 54 mAh g<sup>-1</sup> at 153.6 mA g<sup>-1</sup> calculated per cathode mass. Comparative study has shown that our anode material holds similar excellent performance in both half and full cell configurations. We found that our battery characteristics were determined not only by the used electrode materials, but also by the type of assembled configuration (coin or coffee-bag cell). In this respect, the potential of our cell will be discussed in comparison with other models appearing in the literature.

**Acknowledgement**: This research was supported by NATO Science for Peace and Security (SPS) Programme under grant G5836-SUPERCAR. Authors gratefully acknowledge the financial support from the bilateral project Montenegro-Slovenia "Biomass-derived carbons as anodes in sodium-ion batteries."

# Influence of build orientation and different printing angles on impact toughness of carbon-reinforced PET-G FDM material

<u>Milovan Paunić</u><sup>1</sup>, Aleksandar Sedmak<sup>1</sup>, Milan Janković<sup>1</sup>, Sergiu-Valentin Galaţanu<sup>2</sup>, Horia Dascau<sup>3</sup>, Igor Balać<sup>1</sup> <sup>1</sup>University of Belgrade, Faculty of Mechanical Engineering, Kraljice Marije 16, Belgrade 11120, Serbia <sup>2</sup>Polytechnic University of Timişoara, Department of Mechanics and Strength of Materials, Mihai Viteazu Avenue, Timişoara 300222, Romania <sup>3</sup>ISIM, Mihai Viteazu Avenue, Timişoara 300222, Romania

Carbon-reinforced polyethylene terephthalate glycol (PET-G) material is used in additive manufacturing (AM) for the production of moderately loaded polyester-based parts. Literature review shows that the mechanical properties of these composite materials are substantially influenced by their build orientation regarding printing angle. This paper explores the additional influence of short carbon fibers on the material behavior of composite specimens. In this study, low-energy instrumented Charpy was used as an experimental method for evaluating the impact behavior of material. Experimental evaluation of impact toughness in the case of 3D printed composite specimens with different printing orientation angles (0° and 90°) strongly influence the final mechanical properties of this material. The impact tests were carried out on 5 specimens per batch (a total of 30 specimens). The obtained results from an instrumented pendulum were compared between different specimen groups to have an insight into the influence of build orientation and printing angle on short carbon fiber reinforced PET-G material.

# High-performance hydrophilic separators for supercapacitors based on alkali-modified cellulose nanocrystal aerogels

Daniel Mijailović<sup>1</sup>, Patrick Gane<sup>1,2</sup>, Katarina Dimić-Mišić<sup>2</sup>, Monireh Imani<sup>2</sup>, Dušica Stojanović<sup>1</sup>, Vesna Radojević<sup>1</sup>, Petar Uskoković<sup>1</sup> <sup>1</sup> University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11120 Belgrade, Serbia <sup>2</sup> Department of Bioproducts and Biosystems, School of Chemical Engineering, Aalto University, FI-00076 Aalto, Finland

The shift towards low-carbon technologies is driving an increasing demand for energy conversion and storage systems like supercapacitors, batteries and fuel cells. Therefore, it is crucial to replace traditional materials with renewable and high-performance alternatives. This research introduces a novel approach of designing and fabricating high-performance conductive separators for supercapacitors, leveraging the interaction between alkali ions and highly crystalline nanocellulose (CNC), the most abundant biopolymer. The modified CNC with potassium ions exhibits exceptional performance, surpassing commercial glass microfiber separators in terms of mechanical properties and ionic conductivity. The hydrophilicity and high porosity facilitate efficient potassium ion transport, as demonstrated in supercapacitor devices. By integrating rehydrated conductive separators between glucose-derived mesoporous carbon electrodes, the supercapacitor device achieves high specific capacitance of 80 F/g at 10 mV/s in Swagelok cells and capacitance retention of 95% over 1000 consecutive cycles. These results highlight the potential of these innovative materials to serve as safe and high-performance components in renewable energy storage devices.

#### Crystal structure, x-ray spectroscopic properties and Mössbauer spectra of TaFeP

Ivan Shcherba<sup>1</sup>, Henrik Noga<sup>2</sup>, Victor Antonov<sup>3</sup>, Olga Zhak<sup>1</sup>, Kamila Komedera<sup>2</sup>, Dragan Uskoković<sup>4</sup>, Lev Bekenov<sup>3</sup>, Bohdan Jatsyk<sup>5</sup>, Kateryna Starushenko<sup>1</sup>, Yulija Nykyruy<sup>1</sup> <sup>1</sup>Ivan Franko National University of Lviv, Kyryla & Mefodiya Str. 6, 8, 79-005 Lviv, Ukraine <sup>2</sup>Institute of Technology, University of the NEC, Krakow, Poland <sup>3</sup>G. V. Kurdyumov Institute for Metal Physics of the N.A.S.A., Ukraine <sup>4</sup>Institute of Technical Sciences of SASA, Belgrade, Serbia <sup>5</sup>Lviv National University of Veterinary Medicine and Biotechnologies, Ukraine

The crystal structure of the ternary phosphide TaFeP (TiNiSi-type structure) has been determined from x-ray powder diffraction data: full profile refinement, space group *Pnma*, a = 6.1035 Å, b = 3.5773 Å, c = 6.974 Å,  $R_{int} = 0.0622$ . The genesis of the KB" satellite is well established and illustrated in our numerous works: it reflects the hybridized 3s states of phosphorus in the valence band of transition metal phosphides. When combined in the unified energy scale, the maximum coincides with the main maximum of the  $L_{II,III}$  bands of P. Its intensity depends on the number of P atoms in the nearest environment of the emitting atom and interatomic distances. Our data is sufficient for an unambiguous explanation of the high intensity of the K $\beta$ " satellite: (a) there are 4 P atoms in the nearest environment of Fe; (b) Fe-P distances are abnormally shortened. Examination of the spectra has revealed that in TaFeP the main maximum of the Fe L $\alpha$  band coincides with the high-energy feature of the L<sub>11.11</sub> bands of P, which indicates strong hybridization of P s and Fe d electrons. Mössbauer spectra have been measured at four temperatures in the range 80-300 K. Two components appear in the spectra. Fe1 (77(2) %) and Fe2 (23(2) %). The content of individual components is constant and temperature independent. The paramagnetic component of the spectrum reflects Fe in the crystallographic position 4(c). The moderate value of the quadrupole splitting of 0.3758 mm/s indicates slight anisotropy of the electric field created by Fe1 in the nearest environment. This value is consistent with the previous analysis of the crystal structure. The second component of the Mössbauer spectrum (Fe<sub>2</sub>) can be explained by the coincidence of the high-energy K shoulder of the P spectrum with the main maximum of the Fe d-band, which indicates strong hybridization of P p and Fe d states. At 80 K and 300 K the spectra were measured over a larger speed range to check whether the material has a magnetic component. Theoretical ab initio calculations carried out using the fully relativistic spin-polarized linear muffin-tin orbital method show good agreement with the experimental measurements.

# Determination of optimal conditions of non-linear optical interactions in monoclinic crystals

<u>Anatoliy Andrushchak</u><sup>1</sup>, Dmytro Shulga<sup>1</sup>, Oleg Buryy<sup>1</sup>, Bouchta Sahraoui<sup>2</sup> <sup>1</sup>Lviv Polytechnic National University, Lviv, Ukraine <sup>2</sup>University of Angers, LPhiA, SFRMATRIX, F-49000 Angers, France

As it is known, the highest efficiency of non-linear optical interactions, i.e. second harmonic (SHG), sum frequency (SFG) and difference frequency generation (DFG) in single crystals corresponds to phase matching (PM) condition, in general, represented by the expression  $\vec{k_3} = \vec{k_1} \pm \vec{k_2}$ , where  $\vec{k_1}$ ,  $\vec{k_2}$  are the wave vectors of the input (pump) beams and  $\vec{k_3}$  is the one of the output beam, the upper sign corresponds to SHG or SFG and the lower to DFG. Usually, the case of scalar PM is considered when the directions of pump and output beams wave vectors coincide. However, the general case of vector PM corresponds to a wider variety of possible directions of wave vectors that may lead to the increase of the interaction efficiency in comparison with the scalar case. To reveal the directions of the pump and output beams ensuring the highest efficiencies of non-linear optical interactions, we used the technique based on the construction and analysis of extreme surfaces representing all possible maxima of the considered effect for all possible directions of the output beam. The analysis was performed for biaxial optical crystals of monoclinic symmetry, namely  $GdCa_4O(BO_3)_3$  (GdCOB, point group m), YCa<sub>4</sub>O(BO<sub>3</sub>)<sub>3</sub> (YCOB, point group m), BiB<sub>3</sub>O<sub>6</sub> (BiBO, point group 2) and  $La_2CaB_{10}O_{19}$  (LCB, point group 2) and for different types of PM determined by polarizations of interacting beams. The optimal geometries of vector PM, *i.e.* the directions of wave vectors of the pump and output beams ensuring the highest possible values of the efficiency of intercation were determined. The high enough values of the efficiency increase (in comparison with scalar PM) were revealed for DFG in BiBO crystal – about 80 % for ffs vector PM, where f corresponds to the fast wave and s – to the slow one. Except in this case, the relative increase of the efficiency in the considered monoclinic crystals is usually not higher than 25 %. The obtained results can be used for enhancement of the performance of nonlinear optical devices.

**Acknowledgement**: This research has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 778156 and from Ministry of Education and Science of Ukraine in the frames of 'Nanoelectronics' (0123U101695).

# Carbonization of MOF-5/Polyaniline and ZIF-67/Polyaniline to Zn/N,O-doped and Co/N,O-doped carbon composites with high specific capacitance

<u>Marjetka Savić</u><sup>1</sup>, Aleksandra Janošević Ležaić<sup>2</sup>, Maja Ranković<sup>3</sup>, Nemanja Gavrilov<sup>3</sup>, Igor Pašti<sup>3</sup>, Gordana Ćirić-Marjanović<sup>3</sup>

<sup>1</sup>Vinča Institute of Nuclear Science, University of Belgrade, National Institute of the Republic of Serbia, P.O. Box 522, 11001 Belgrade, Serbia

<sup>2</sup>University of Belgrade-Faculty of Pharmacy, Vojvode Stepe 450, 11221 Belgrade, Serbia <sup>3</sup>University of Belgrade-Faculty of Physical Chemistry, Studentski trg 12-16, 11158 Belgrade, Serbia

Composites of metals, metal oxides and metal sulfides with carbons are very interesting materials due to their various applications in the field of energy conversion and energy storage. For this purpose, two carbon composites were synthesized by direct carbonization of two precursor composites of polyaniline in conductive emeraldine salt form (PANI-ES), and metal-organic frameworks, MOF-5 and ZIF-67. The PANI component served as a source of N heteroatoms, while MOF-5 and ZIF-67 were sources of Zn and Co, respectively, in derivatives obtained by carbonization. Both precursor composites were made by mechanochemical method mixing with pestle in a mortar measured amounts of PANI-ES and MOF-5 or ZIF-67 in until complete solvent evaporation.

Direct carbonization of composite precursors MOF-5/PANI and ZIF-67/PANI was performed up to the temperature of 800 °C in an argon environment. New materials were characterized in order to examine their structural and textural characteristics (FTIR, and Raman spectroscopy, SEM-EDX, XRD, conductivity and N<sub>2</sub> sorption measurements). Products of carbonization, C(MOF-5/PANI) and C(ZIF-67/PANI), represent composites of N,O-doped carbons with ZnO/ZnS and Co-containing phases, respectively. Cyclic voltammetry was used to evaluate their electrochemical behavior, especially with the aim of assessing the charge storage ability and measuring the specific capacitance,  $C_{\text{spec}}$ . Cyclic voltammograms were measured in an alkaline (6 M KOH) electrolytic solution at various potential sweep rates (v) from 10 to 200 mV s<sup>-1</sup>. The composite C(MOF-5/PANI) showed much higher  $C_{\text{spec}}$  (238.2 F g<sup>-1</sup> at v = 10 mV s<sup>-1</sup>) than the composite C(ZIF-67/PANI) (88.48 F g<sup>-1</sup> at v = 10 mV s<sup>-1</sup>). Electrochemical results can be explained by the larger porosity of MOF-5 than ZIF-67 in the precursors, resulting in a more developed pore structure of C(MOF-5/PANI).

# Oxidation resistance and electrical conductivity of nanostructured coatings for titanium interconnects of solid oxide fuel cell

Viktoriya Podhurska<sup>1</sup>, Orest Ostash<sup>1</sup>, Mykola Kuzmenko<sup>2</sup>, Oleksander Kuprin<sup>3</sup> <sup>1</sup> Karpenko Physico-Mechanical Institute of the NAS of Ukraine, Lviv, Ukraine <sup>2</sup> Institute for Problems of Materials Science of the NAS of Ukraine, Kyiv, Ukraine <sup>3</sup> National Science Center "Kharkiv Institute of Physics and Technology" of the NAS of Ukraine, Kharkiv, Ukraine

Nowadays, solid oxide fuel cells (SOFCs), which at temperatures of 600-800 °C convert the chemical energy of the interaction of hydrogen or hydrocarbons with air oxygen into electrical energy with an efficiency of 65 to 70 %, are used as means of alternative energy. Interconnects, which provide the supply of the operating gas environment and current transportation in fuel cell stacks, serve as their multifunctional components. An interconnect significantly overcomes the anode, electrolyte, and cathode in terms of weight; therefore, it determines the weight of the stack, which can reach hundreds of kilograms. Interconnect materials should possess high physical and mechanical characteristics. As materials for interconnects, highly alloyed steels, with oxidation resistant and electrically conductive coatings based on spinel or perovskite are traditionally used. However, such interconnects lead to a significant weight of the stacks (the density of steel is 7.8 g/cm<sup>3</sup>). The use of titanium alloys and composites, especially based on titanium MAX phases, will make it possible to create interconnects for lighter SOFC stacks (by ~ 2 times), since these materials have a density of 3.9-4.5 g/cm<sup>3</sup>.

The aim of the work is to study the service properties of thin (0.5 mm) titanium interconnects made of the Ti-Al-Mn system alloy with nanostructured coatings of the Ti-Al-Zr-Sn-Si-Mo-Nb-Mn system SOFC at 600  $^{\circ}$ C in the air.

The coatings were deposited on polished Ti-Al-Mn system alloy specimens using a Ti-Al-Zr-Sn-Si-Mo-Nb-Mn cathode and PVD method. Oxidation resistance and electrical conductivity of coatings after long-term (1000 h) holding at 600 °C was 0.75 to 85 mg/cm<sup>2</sup>. Electrical conductivity of obtained coating was  $3.5 \cdot 10^5$  S/m.

### Waterborne polyurethane nanocomposite reinforced by chitin glucan nanocrystals

Beata Strachota, Silvia Mares Barbosa, Adam Strachota, Ewa Pavlova, Magdalena Konefał, Jiří Hodan Institute of Macromolecular Chemistry, Czech Academy of Sciences, Heyrovského nám. 2, 162 00 Praha 6, Czech Republic

Chitin is a widely available natural polymer and is the primary structural component of crustacean shells and the cell wall of fungi. Besides strong hydrogen bonding ability, it possesses two highly desirable properties: biocompatibility and biodegradability. Its complex with glucan (ChGC), which can be isolated from fungi, has numerous health benefits, including anti-inflammatory, antioxidant and anticancer effects. This study introduces novel elastomers synthesized from a waterborne polycarbonate-based polyurethane dispersion, which are reinforced by chitin-glucan nanocrystals (ChGNCs). Utilizing an environmentally friendly method, aqueous solutions of polyurethane prepolymer dispersion and ChGNCs were blended, followed by gradual water evaporation, which yielded the nanocomposite elastomers.

The studied nanofiller, the chitin-glucan complex from Aspergillus Niger, was defibrinated dried micellium. An acidic deep eutectic solvent mixture (DES) was used to isolate the ChGNCs. This disintegration of naturally occurring chitin bundles into ChGNCs leads to nanofillers with very high aspect ratios.

The incorporation of high-aspect-ratio hydrogen-bonding ChGNCs into polycarbonate-PUR distinctly improves the mechanical properties and the thermal stability of the nanocomposite elastomers. This contribution focuses on the characterization of PUR nanocomposite films using advanced characterization techniques, including micro-stretch tests, as well as relaxation and self-assembly tests. The morphology of the products was investigated by X-ray scattering and electron microscopy.

The study highlights the potential of natural and biological raw materials, combined with organic-solvent-free processes, to fulfil rigorous quality standards in biomedical and tissue engineering applications. Furthermore, this innovative approach accelerates the development of materials with improved mechanical properties.

*Acknowledgement*: The authors would like to acknowledge the financial support from the Ministry of Education Youth and Sports of the Czech Republic (Grant LUAUS23004).

# Facile synthesis of CoAu/rGO nanocomposite for sensing of As<sup>3+</sup> ions in neutral medium

<u>Kristina Radinović</u><sup>1</sup>, Jadranka Milikić<sup>1</sup>, Nemanja Gavrilov<sup>1</sup>, Dalibor Stanković<sup>2</sup>, Aleyna Basak<sup>3</sup>, Önder Metin<sup>3,4</sup>, Biljana Šljukić<sup>1,5</sup>

<sup>1</sup>University of Belgrade, Faculty of Physical Chemistry, Studentski trg 12-16, 11158 Belgrade, Serbia
 <sup>2</sup>University of Belgrade, Faculty of Chemistry, Studentski trg 12-16, 11158 Belgrade, Serbia
 <sup>3</sup>Department of Chemistry, College of Sciences, Koç University, 34450 Istanbul, Türkiye
 <sup>4</sup>Koç University Surface Science and Technology Center (KUYTAM), 34450 Sarıyer, Istanbul, Türkiye
 <sup>5</sup>Center of Physics and Engineering of Advanced Materials, Laboratory for Physics of Materials and Emerging Technologies, Chemical Engineering Department, Instituto Superior Técnico, Universidade de Lisboa, 1049–001 Lisbon, Portugal

Arsenic is a heavy metal present in the earth's crust and groundwater in different organic and inorganic forms. The inorganic forms are reported to be more toxic than the organic forms because they can react with enzymes in the human and animal body. Of the inorganic forms of arsenic (-3, 0, +3, and +5), it is reported that  $As^{3+}$  is *ca*. 60 - 70 times more toxic than  $As^{5+}$  [1]. Herein, we synthesized bimetallic CoAu nanoparticles on reduced graphene oxide (rGO), as well as monometallic counterparts Co/rGo and Au/rGO, and subsequently investigated them for the electrochemical detection of  $As^{3+}$  in 1 mM NaAsO<sub>2</sub> at pH 7 by anodic stripping voltammetry. The voltammogram of the CoAu/rGO electrode evidences its activity for the detection of  $As^{3+}$  in 1 mM NaAsO<sub>2</sub> solution, *i.e.* it shows a well-defined peak corresponding to the electrooxidation of  $As^{0}$  to  $As^{3+}$ . The detection limit of  $As^{3+}$  ions using the CoAu/rGO electrode was calculated to be as low as  $4.5\pm0.1$  ppb which is significantly lower than the maximum limit value of the World Health Organization (10 ppb) for As ions in water. Studies of long-term stability and life-time of the CoAu/rGO electrode are ongoing.

# **Reference:**

 Radinović, K.; Milikić, J.; Santos, D.M.F.; Saccone, A.; De Negri, S.; Šljukić, B. Electroanalytical sensing of trace amounts of As(III) in water resources by Gold-Rare Earth alloys. J. Electroanal. Chem. 2020, 872, 114232. <u>https://doi.org/10.1016/j.jelechem.2020.114232</u>.

# Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXenes: enhancing performance in glucose biosensors

<u>Anton Popov<sup>1,2</sup></u>, Viktorija Lisyte<sup>2</sup>, Marina Sapauskiene<sup>2</sup>, Asta Kausaite-Minkstimiene<sup>1,2</sup>, Almira Ramanaviciene<sup>1,2</sup>

<sup>1</sup>Department of Immunology and Bioelectrochemistry, State Research Institute Centre for Innovative Medicine, Vilnius, Lithuania

<sup>2</sup>NanoTechnas - Center of Nanotechnology and Materials Science, Faculty of Chemistry and Geosciences, Vilnius University, Vilnius, Lithuania

Diabetes presents as a chronic metabolic condition characterized by disrupted glucose regulation. The global incidence of diabetes in adults has surged significantly, escalating from 108 million in 1980 to 463 million by 2019. While current glucose biosensors are adept at detecting glucose levels in blood, developing non-invasive or more sensitive biosensors poses a challenge. Leveraging nanomaterials holds promise for enhancing the analytical capabilities of glucose biosensors.

MXenes, a recently identified class of 2D nanomaterials comprising transition metal carbides and nitrides. Their potential application in biosensors is enticing due to their nearly metallic conductivity, distinct optical properties, modifiable surface chemistry, and inherent hydrophilicity, among other attributes.

This study focuses on utilizing  $Ti_3C_2T_x$  MXenes to fabricate a glucose biosensor. We optimized MXenes and glucose oxidase deposition on the electrode surface and explored various electron transfer mediators to enhance biosensor performance. In addition, the performance of the developed biosensor was evaluated.

Acknowledgment: This project has received funding from the Research Council of Lithuania (LMTLT), agreement No S-PD-24-4.

# Niobium MXenes with lanthanum: electrochemical performance in microsupercapacitors

<u>Meriene Gandara</u><sup>1</sup>, Bianca Fortes Palley<sup>1</sup>, Lazar Rakočević<sup>2</sup>, Dušan Mladenović<sup>3</sup>, Biljana Šljukić<sup>3,4</sup>, Emerson Sarmento Gonçalves<sup>1,5</sup> <sup>1</sup>Technological Institute of Aviation, Space Science and Technology Graduate Program, Praça Marechal Eduardo Gomes, 50,12228-900, São José dos Campos, Brazil <sup>2</sup>Vinča Institute of Nuclear Sciences, Department of Atomic Physics, 12-14 Mike Petrovića Street, Belgrade, Serbia

<sup>3</sup>University of Belgrade, Faculty of Physical Chemistry, Studentski trg 12-16, 11158 Belgrade, Serbia <sup>4</sup>Center of Physics and Engineering of Advanced Materials, Laboratory for Physics of Materials and Emerging Technologies, Chemical Engineering Department, Instituto Superior Técnico, University of Lisbon, Portugal

<sup>5</sup>Institute of Aeronautics and Space, Materials Department, Praça Marechal Eduardo Gomes, 50 e 12228-904, São José dos Campos, Brazil

The introduction of different elements into 2D materials was proven to be a successful strategy for tuning their physicochemical properties [1]. For application in energy storage devices, inserting heteroatoms into the MXene structure adjusts the interlayer structure and surface area, increases the stability and electrochemical performance, significantly reducing resistance to charge transfer [2]. In this work, Nb MXene was obtained by using the MILD etching process of the Nb MAX phase. The obtained MXene was further subjected to 1 M La(NO<sub>3</sub>)<sub>3</sub> solution at 80 °C for 4h. Nb MXene with La (Nb-MX/La) was characterized by SEM/FEG with EDS, XRD analysis and XPS, and its electrochemical properties by CV, EIS and GCD in 1 M H<sub>2</sub>SO<sub>4</sub>. Nb-MX/La delivered specific power of 37.5 mW cm<sup>-2</sup> and specific energy of 10.62  $\mu$ Wh cm<sup>-2</sup> at 50 mA cm<sup>-2</sup>, capacitance retention of 133 % and coulombic efficiency of 101 % after 1000 cycles. Therefore, the material presented electrochemical characteristics applicable to electrodes of microsupercapacitor devices.

### **References:**

- 1. Wang, X.; Sun, G.; Routh, P.; Kim, D.-H.; Huang, W.; Chen. P. *Chem. Soc. Rev.* Heteroatom-doped graphene materials: syntheses, properties and applications. **2014**, *43*, 7067–7098.
- Dey, A.; Varagnolo, S.; Power, N.P.; Vangapally, N.; Elias, Y.; Damptey, L.; Jaato, B.N.; Gopalan, S.; Golrokhi, Z.; Sonar, P.; Selvaraj, V.; Aurbach, D.; Krishnamurthy, S. Doped MXenes—a new paradigm in 2D systems: synthesis, properties and applications *Prog. Mater. Sci.* 2023, 139, 101166.

# Microstructural transformation of SPD processed Al-Li alloys during low temperatures deformation

<u>Sergii Shumilin</u><sup>1</sup>, Tetiana Hryhorova<sup>1</sup>, Pavel Zabrodin<sup>1,2</sup>, Daria Drozdenko<sup>3</sup> <sup>1</sup> B. Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine, 47 Nauky Ave., Kharkiv, 61103, Ukraine

<sup>2</sup>Czech Academy of Sciences, Institute of Theoretical and Applied Mechanics, Prosecka 809/76, 190 00 Prague, Czech Republic

<sup>3</sup>Charles University, Faculty of Mathematics and Physics, Department of Physics of Materials, Ke Karlovu 5, Prague, 121 16, Czech Republic

The work was focused on studying the microstructure evolution of an ultrafine-grained Al-3.8 at.% Li alloy prepared by equal-channel angular hydroextrusion. The mechanical properties of the samples were determined during uniaxial tension in the temperature range 4.2 to 400 K.

The results demonstrated that temperature has a significant impact on the plasticity and strength of the alloy. A comprehensive analysis of the microstructure focused on the evolution of grain size, texture, and dislocation structure has been performed. It was determined that the microstructure after tension exhibits an elongated structure in the loading direction. The microstructure of the sample deformed at 400 K differs from the rest of the samples deformed at lower temperatures and characterized by a high density of high-angle grain boundaries and low internal deformations. This indicates the dislocation annihilation processes. The samples after deformation at lower temperatures are characterized by high internal deformations and a high density of low-angle grain boundaries. Furthermore, there is a tendency for the density of geometrically necessary dislocations (GND) to increase with a decrease in the deformation temperature. The accumulation of dislocations during deformation in the temperature range of 140-295 K leads to rapid localization of deformation and failure (elongation to failure of 3 to 7%). With a further decrease in the deformation temperature, the density of GND increases. However, the higher density of accumulated GNDs during deformation below 100 K does not lead to localization and premature failure. Consequently, an increase in ductility appeared during deformation at 4.2 K (elongation to failure of 25 %).

# Nanoscale assessment of free volume in BaGa<sub>2</sub>O<sub>4</sub> ceramics doped with Eu<sup>3+</sup> ions using PAL spectroscopy

<u>Halyna Klym</u><sup>1</sup>, Yuriy Kostiv<sup>1</sup>, Oleksii Kushnir<sup>2</sup> <sup>1</sup>Lviv Polytechnic National University, Lviv, Ukraine <sup>2</sup>Ivan Franko National University of Lviv, Lviv, Ukraine

The  $BaGa_2O_4$  ceramics represent a promising material for various applications, including insulation in optoelectronic devices and as a secondary coating for plasma panels. The introduction of impurities, particularly rare-earth ions, into these ceramics enhances their functional properties. This study aims to investigate the evolution of nanoscale inner free volumes in  $BaGa_2O_4$  ceramics doped with varying amounts of  $Eu^{3+}$  ions using positron annihilation lifetime spectroscopy (PAL). The evolution of free volume defects in BaGa<sub>2</sub>O<sub>4</sub> ceramics, synthesized via solid phase synthesis from BaCO<sub>3</sub> and Ga<sub>2</sub>O<sub>3</sub> components with different concentrations of  $Eu_2O_3$  (1, 3, and 4 mol.%), was examined. PAL measurements were conducted using the ORTEC system with a <sup>22</sup>Na isotope as the positron source. The PAL spectra were analyzed using a four-component fitting procedure tailored for spinel ceramics with a branched porous structure. In BaGa<sub>2</sub>O<sub>4</sub> ceramics, two PAL channels were identified: the capture of positrons by bulk defects with short and medium lifetimes, and the decay of orthopositronium atoms with long lifetimes. The short-term component reflects microstructural features of the main phase, while the middle component is associated with defect-related voids near grain boundaries. The lifetimes of the third and fourth long-term components are indicative of nanopore transformation. Additional phases in the ceramics are predominantly localized near grain boundaries, serving as defective centers for positron capture as observed through PAL spectroscopy. Analysis of the second component of the PAL spectra for both undoped and Eu<sup>3+</sup>-doped BaGa<sub>2</sub>O<sub>4</sub> ceramics revealed that an increase in the Eu<sup>3+</sup> content from 1 to 3 mol.% results in an agglomeration of free volume defects near grain boundaries. Concurrently, the nanopores in the ceramics expand, and their number increases. Further increments in the Eu<sup>3+</sup> ion content led to fragmentation of both free volume defects and nanopores.

#### 25<sup>th</sup> YUCOMAT 2024 & XIII WRTCS Herceg Novi, September 2 - 6, 2024

# P.S.III.D.7

# Modification of ZnO surfaces with oxygen vacancies: density functional study

Jelena Belošević-Čavor, Vasil Koteski, Valentin Ivanovski, Ana Umićević, Dragan Toprek, Ana Kapidžić Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade,

Belgrade, Serbia

ZnO is a complex material, whose properties are very sensitive to preparation conditions due to the presence of various intrinsic defects. Using the modified density functional calculations, we study the relative stability of the nonpolar  $(10\underline{1}0 \text{ and } 11\underline{2}0)$  and the polar (zinc-terminated  $(000\underline{1})$ -Zn and oxygen-terminated  $(000\underline{1})$ -O) ZnO surfaces, as well as the influence of oxygen vacancies on their stability and electronic structure. In our study we consider models of surfaces with different positions and concentrations of oxygen vacancies. Particular attention is given to the charge state of the oxygen vacancies and charges of the individual atoms. We find that the 1010 surface is the most stable, while the polar (0001)-Zn surface is the least stable. Our calculations indicate that the configuration with oxygen vacancies at the top of the surface is the most favorable for all studied surfaces. The obtained results for the structural relaxations and energetics are compared with previous theoretical and experimental data.

Acknowledgment: This research was supported by the Science Fund of the Republic of Serbia, The Program PRISMA, #7377, Water pollutants detection by ZnO-modified electrochemical sensors: From computational modeling via electrochemical testing to real system application – WaPoDe.

### P.S.III.D.8

# Swelling behaviour and heavy metals adsorption on alginate-based hydrogels filled with LaponiteRD and montmorillonite

<u>Olena Goncharuk</u><sup>1,2</sup>, Nataliia Guzenko<sup>1</sup>, Yurii Samchenko<sup>2</sup>, Svitlana Dybkova<sup>2</sup>, Katarzyna Szewczuk-Karpisz<sup>1</sup>

<sup>1</sup>Institute of Agrophysics, Polish Academy of Sciences, Doświadczalna 4, 20-290 Lublin, Poland <sup>2</sup>Ovcharenko Institute of Biocolloidal Chemistry of NAS of Ukraine, 42 Vernadskogo Blvd., Kyiv, 03142, Ukraine

The development of bio-safe, effective and multifunctional materials for eco-applications, such as removal of toxic contaminants from soil or water, is a high demand trend in recent years. Composite hydrogel materials based on sodium alginate showed great potential in relation to the sorption of heavy metal ions and organic pollutants. In addition, by adjusting the swelling degree of such composites, it is possible to increase the water-retaining properties when applying them as soil conditioners. As part of the work, a series of alginate-based hydrogels were synthesized using CaCl<sub>2</sub> as a crosslinking agent. Montmorillonite and LaponiteRD were used as fillers to control mechanical strength, swelling and sorption properties. The biosafety of the synthesized hydrogels was determined by assessing their genotoxicity according to the comet method and by Nelyubov test. It is shown that the degree of swelling and the sorption capacity in relation to Cd(II) and Fe(II) ions decrease exponentially with an increase in the degree of crosslinking by Ca<sup>2+</sup> and decrease monotonously with an increase in clay concentration in composites. The concentration of the CaCl<sub>2</sub> in the range of 0.3-0.5 wt. % was chosen as optimal for synthesis of mechanically strong hydrogels with a high swelling degree. For a series of alginate/clay hydrogels, sorption properties in relation to Cd(II) and Fe(II) were studied. It was established that the sorption capacity decreases with an increase in clay and crosslinking agent concentration, and the affinity of the hydrogels is higher in relation to Cd(II) (up to 1.31 mmol/g) than to Fe(II) (up to 0.92 mmol/g), and the amount of sorbed metal ions affects the swelling degree of hydrogels, due to additional cross-linking their structure.

*Acknowledgments*: The authors are grateful for the financial support by Polish Academy of Sciences and U.S. National Academy of Sciences (Agreement No. PAN.BFB.S.BWZ.331.022.2023 «Biocompatible hybrid hydrogels with functional inorganic fillers for strengthening of plant vegetation»).

### P.S.III.D.9

# Sky Harvesting with Sustainable Materials: NO<sub>x</sub> Mitigation through Air Mining applying Ambient Air Pollution Simulation and Kinetic Modelling

<u>Nemanja Barać</u><sup>1</sup>, Katarina Dimić-Mišić<sup>2</sup>, Mirko Stijepović<sup>3</sup>, Mirjana Kijevčanin<sup>3</sup>, Monireh Imani<sup>2</sup>, Petar Uskoković<sup>3</sup>, Đorđe Janaćković<sup>3</sup>, Ernesto Barceló<sup>2,4</sup>, Patrick Gane<sup>2,3</sup> <sup>1</sup>Innovation Center of Faculty of Technology and Metallurgy in Belgrade Ltd., Karnegijeva 4, 11000 Belgrade, Serbia

<sup>2</sup>School of Chemical Engineering, Department of Bioproducts and Biosystems, Aalto University, 00076 Aalto, Helsinki, Finland

<sup>3</sup>Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11000 Belgrade, Serbia
 <sup>4</sup>Environmental, Social and Governance, Gestamp Automoción S.A., Torre Ombú nº3, Planta 1, 28045 Madrid, Spain

Previously developed sustainable materials were used in the form of filter sheets designed to meet circular economy criteria by (i) initiating a cycle for employing a filter substrate made of over-recycled natural cellulose fibres, (ii) engaging micro-nanofibrillated cellulose (MNFC) derived from the same cellulose fibres as binder and control humectant, (iii) adopting a naturally re-generated mineral, limestone, and finally (iv) following exposure to NO<sub>x</sub>, forming a product of added value having further functionality rather than being itself a waste product. The use of CaCO<sub>3</sub> for NO<sub>x</sub> collection and storage in the presence of atmospheric moisture is advantageous because it stores the polluting gas beyond surface saturation levels through a conversion reaction rather than pure adsorption. The conversion reaction transforms gaseous NO<sub>x</sub> into a stable nitrogen species in the form of calcium nitrate salt. As a focal point in current industrial practices aimed at advancing the circular economy, the nitrate-rich CaCO<sub>3</sub>-cellulose-based filter can be repurposed post-use as a soil fertilizer and micronutrient, exemplifying sustainable material sourcing before and after initial use. This application of air mining technology holds promise as a sustainable solution for reducing air pollution and supporting agriculture through the use of sustainable materials.

In the current research on this topic, a simulation of increased ambient pollution with NO<sub>2</sub> gas was conducted to obtain experimental data on the yield of nitrites and nitrates on filter papers under various ambient conditions. The exposure was carried out using an air conditioning chamber at different temperatures and humidity levels. Initial results indicate that rising temperatures and humidity levels in the air, while maintaining a constant concentration of NO<sub>2</sub> gas, lead to an increase in the concentration of nitrate and nitrite ions formed on the filter sheets. The goal we set in this practical example was to evaluate and select a kinetic model for analysing experimental data. This involved comparing various alternatives based on adsorption experiments, which included chemical reactions occurring under specific hydrodynamic conditions over porous or topographical adsorbent media. By combining experimental results from exposing and saturating filter sheets with gaseous phase adsorption and conversion into several kinetic models, we established satisfactory criteria for determining the most reliable mathematical equations and parameters. This approach enabled accurate prediction of the chemical kinetics, effectively reproducing the experimental results from our setup.

Acknowledgement: The research was supported by Omya International AG, Group Sustainability, Switzerland.

# Novel Hybrid Poly(methacrylic acid)/Gelatin/Alginate Hydrogels for Bone and Cartilage Tissue Engineering

<u>Vukašin Ugrinović</u><sup>1</sup>, Maja Marković<sup>1</sup>, Vesna Panić<sup>1</sup>, Đorđe Veljović<sup>2</sup> <sup>1</sup>Innovation Center of Faculty of Technology and Metallurgy, Belgrade, Serbia <sup>2</sup>Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia

Hydrogels, characterized by their hydrophilic, porous, and permeable nature, have been extensively studied for biomedical applications due to their tissue-mimicking properties. This study introduces novel poly(methacrylic acid) (PMA)/gelatin/alginate hydrogels synthesized through combined processes of free-radical polymerization and freeze-drying, offering adjustable mechanical, morphological, and biological characteristics akin to human cartilage. The ratio of PMA to gelatin played a critical role, influencing mechanical strength, morphology, and biological response. Incorporating alginate slightly decreased mechanical properties while increasing porosity and water content. However, subsequent crosslinking with therapeutic ions such as Ca<sup>2+</sup> and Mg<sup>2+</sup> had a more pronounced effect in hydrogels with higher alginate content, enhancing mechanical properties and reducing porosity. Compared to single network PMA hydrogels, our hybrid network hydrogels demonstrated significantly improved compressive strength, modulus, and fatigue resistance. Additionally, these hydrogels exhibited excellent fatigue resistance and biocompatibility, positioning them as promising candidates for biomedical applications.

**Acknowledgements:** This research was funded by the Science Fund of Republic of Serbia #GRANT No.7470, Novel hybrid biomimetic macroporous composites with tuned biodegradability, improved osteointegration and anticancer properties for bone tissue regeneration – HyBioComBone and by Ministry of Science, Technological Development and Innovations, Republic of Serbia (No. 451-03-65/2024-03/200135, 451-03-66/2024-03/200287)

#### Acrylate functional composites reinforced using the ZnAl layered double hydroxide

Marija Jovanović<sup>1</sup>, Vladislav Tadić<sup>1</sup>, Marija Vuksanović<sup>2</sup>, Miloš Petrović<sup>1</sup>, Vesna Radojević<sup>1</sup>, <u>Radmila Jančić Heinemann</u><sup>1</sup> <sup>1</sup>Faculty of Technology and Metallurgy, University of Belgrade <sup>2</sup>Vinca Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belarade

Layered structures have great interest in the research of composite materials as they enable the tunning of the materials properties when used as reinforcement. As they can express several functional uses, they are the choice for functional composite materials. Layered double hydroxides are one of the layered structural materials that can be synthesized in a simple way using coprecipitation in laboratory experiments and their properties can be adjusted using the synthesis paths that are easily controlled in the process. Zinc compounds are known to have inhibiting influence on the development of microbial species, and they are a choice in some situations when the material must be resistant to microbial attack.

Dentures and dental apparatus for corrections for children tooths are materials that are produced from the PMMA and they stay in contact with the patient for a long time. Microcracks arise in those composites, and they are an open route for bacteria to develop. Adding the zinc compound as a reinforcement could decrease this possibility and at the same time, improve the mechanical properties of the material.

ZnAl layered hydroxide will be synthesized in coprecipitation process and used as reinforcement in the composite having PMMA as a matrix. Tensile properties and toughness are tested. Addition of the reinforcement in form of layered double hydroxide improves composite mechanical properties compared to the matrix itself.

# Ti<sub>3</sub>C<sub>2</sub> MXene-Based Electroconductive Polymer Nerve Guidance Conduits for Regeneration of Peripheral Nerve Injuries

Inna Chorna<sup>1</sup>, Sergiy Kyrylenko<sup>1</sup>, Kateryna Diedkova<sup>2</sup>, Zhanna Klishchova<sup>1,3</sup>, Serhii Dukhnovskiy<sup>4</sup>, Ivan Baginskiy<sup>4</sup>, Veronika Zahorodna<sup>4</sup>, Iryna Roslyk<sup>4</sup>, Oleksiy Gogotsi<sup>4</sup>, Paola Caro<sup>5</sup>, Alexandre Oliveira<sup>5</sup>, Maksym Pogorielov<sup>1,2</sup> <sup>1</sup>Biomedical Research Center, Sumy State University, Sumy, Ukraine <sup>2</sup>Institute of Atomic Physics and Spectroscopy, University of Latvia, Riga, Latvia <sup>3</sup>Federal University of Lavras UFLA, Lavras, MG, Brazil <sup>4</sup>Carbon Ukraine Ltd, Kyiv, Ukraine; <sup>5</sup>University of Campinas UNICAMP, Campinas, SP, Brazil

Injuries to peripheral nerves present a substantial public health challenge, exacerbated by increased travel frequency and a regrettable rise in armed conflicts. The gold standard surgical technique involves utilizing nerve autografts, resulting in additional injury at the donor site. Nerve guidance conduits (NGC) are specialized structures designed to facilitate the repair of damaged nerves. NGCs require new polymeric biomaterials that are biocompatible, biodegradable, and supportive.

Given the electrical nature of neuronal signals, it has been proposed to utilize electroconductive conduits to enhance the efficacy of regeneration. However, most polymers are dielectrics. MXenes, a novel family of 2D nanomaterials with exceptional properties, can be used to render the polymer NGCs conductive. The non-toxic and biocompatible nature of MXenes makes them ideal candidates for designing the next-generation NGCs.

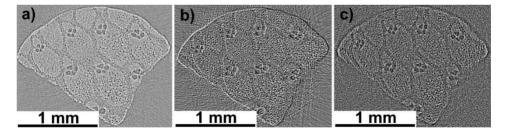
Therefore, our project focuses on developing polymer nanofibrous membranes coated with  $Ti_3C_2$  MXene. These membranes are utilized to construct neural guidance conduits to address sciatic nerve injury in rats. We also address the fate of MXene after prolonged incubation in the animal's body using transmission electron microscopy. While the project is ongoing, we have already observed enhanced functional recovery in the injured paw treated with the MXene-based nerve guidance conduits.

Acknowledgements: Supported by the Air Force Office of Scientific Research via EOARD project P809, HORIZON-MSCA-2022-SE-01-01 project #101131147 ESCULAPE, LRC grant #2023/1-0243, grant #3050 of the EURIZON H2020 project 871072, CAPES project #23038.003877/2022-44 SOLIDARIEDADE ACADÊMICA, project #0124U000637 of the Ministry of Education and Science of Ukraine, ERASMUS-JMO-2022-CHAIR project #101085451 CircuMed, ERASMUS-JMO-2023-MODULE project #101127618 MedFood.

## In-line X-ray phase-contrast imaging of a bamboo splinter

Pavel Zabrodin<sup>1,2</sup>, Daniel Vavřík<sup>1</sup>, Pavel Beneš<sup>1</sup>, Jan Žemlička<sup>3</sup> <sup>1</sup>The Czech Academy of Sciences, Institute of Theoretical and Applied Mechanics, Praha, Czech Republic <sup>2</sup> B. Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine, Kharkiv, Ukraine <sup>3</sup>Institute of Experimental and Applied Physics, Czech Technical University in Prague, Praha. Czech Republic

One of the inherent limitations of X-ray microcomputed tomography (X $\mu$ CT) is its low sensitivity to the visualization of subtle alterations in density. Various X-ray phase contrast imaging (XPCI) techniques are applied to enhance the sensitivity of visualization of materials due to their differing refractive index. Some of these are laboratory-based methods that require complex equipment that reduces photon energy and limits their use on massive samples. The In-line XPCI method of algebraically identifying the phase component has no such limitation and assumes the contrast observed during XuCT can be attributed to both absorption and object-induced phase shift. To develop an in-line approach to the algebraic extraction of the phase component from XuCT data, the study examined the efficacy of a range of frequency filtering techniques, evaluated across both the spatial and frequency domains, in conjunction with noise reduction strategies at various processing stages. As an object and a standard, the data from [1] on absorption grating-based (GB) XPCI with a hybrid pixel detector Timepix, were used. The results demonstrated the efficacy of the following approach: firstly, the absorption projections (a) were filtered in the frequency domain using a low-pass Butterworth filter; secondly, the MLVUM method [2], based on adaptive Gaussian filtering, was applied, followed by further Filtered Back Projections reconstruction. The proposed processing method applies to in-line XPCI, as evidenced by the correlation between the GB XPCI data (b) and the data obtained in this study (c).



#### **References:**

- 1. J. Zemlicka et al., Journal of Instrumentation, 2019, 14, C05007.
- 2. D. Edla et al., Journal of Digital Imaging, 2022, 35, 1041-1060.

# The corrosion resistance of the nanostructured modified ultrafine-grained titanium in Ringer's solution

Dragana Mihajlović<sup>1</sup>, Jelena Bajat<sup>1</sup>, Veljko Đokić<sup>1,2</sup>

<sup>1</sup>University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11120 Belgrade, Serbia <sup>2</sup>Innovation Centre of Faculty of Technology and Metallurgy, Karnegijeva 4, 11120 Belgrade, Serbia

To optimize corrosion resistance, as one of the important factors for biocompatibility of the metallic implants, the titanium-based materials can be modified by different treatments, including severe plastic deformation (SPD) and anodic oxidation. In the present study, oxide layer on the surface of ultrafine-grained titanium (UFG cpTi) was formed using anodic oxidation in 1 M  $H_3PO_4$  + NaF solution, at room temperature for 60 minutes. The nanotubes morphology was studied using field emission scanning electron microscopy (FESEM). The FESEM microphotographs showed that anodic oxidation of ultrafine-grained titanium in the selected solution can lead to the formation of a highly regular oxide layer with nanotubes. This study aimed to determine the corrosion resistance of titanium after high-pressure torsion (HPT) and anodic oxidation. Corrosion resistance was tested in Ringer's solution with a pH value of 5.5 at 37 °C, in order to simulate the environment in the human body. The ultrafinegrained titanium, before and after anodic oxidation, was analyzed by electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization. The inner barrier and outer porous surface layers were highly resistant with capacitive behaviour, but the ultrafine-grained titanium with an oxide layer with nanotubes on the surface showed improved corrosion resistance.

# Si-modified biogenic hydroxyapatite/alginate hydrogel composites: structure and properties

Yuri Samchenko<sup>1</sup>, <u>Olena Sych<sup>2,3</sup></u>, Nataliia Pinchuk<sup>2,4</sup>, Liudmyla Kernosenko<sup>1</sup>, Svitlana Stelmakh<sup>3</sup>, Jan Mizeracki<sup>3</sup>, Pavlo Vorotytskyi<sup>1</sup>, Tetiana Poltoratska<sup>1</sup>, Anna Synytsia<sup>2</sup>, Ganna Chyzhyk<sup>5,7</sup>, Yuliia Vronska<sup>6,7</sup>
 <sup>1</sup>F.D. Ovcharenko Institute of Biocolloidal Chemistry of NAS of Ukraine, Kyiv, Ukraine
 <sup>2</sup>Frantsevich Institute for Problems of Materials Science of NAS of Ukraine, Kyiv, Ukraine
 <sup>3</sup>Institute of High Pressure Physics of the PAS, Warsaw, Poland
 <sup>4</sup>Institute of Low Temperature and Structure Research of the PAS, Wrocław, Poland
 <sup>5</sup>G.S. Pisarenko Institute for Problems of Strength of NAS of Ukraine, Kyiv, Ukraine

<sup>7</sup>Institute of Metallurgy and Materials Science of the PAS, Krakow, Poland

The development of injection materials for orthopedics and traumatology is extremely relevant today, as it allows minimizing surgical procedure. Alginate-based injectable hydrogels have held the attention of researchers due to their significant biomedical potential and unique properties. Biogenic hydroxyapatite (BHA) preserves the natural nanostructure of the mineral matrix of bone tissue and shows the efficiency and prospects for bone treatment. In this study, Si-modified biogenic hydroxyapatite/alginate hydrogel composites were prepared by ionic crosslinking with different amount of inorganic component (1, 2, 3 %), which contains 2 wt.% and 5 wt.% silicon. XRD, FTIR, SEM, helium pycnometry as well as the swelling study were used for composites characterization. XRD and FTIR confirmed the presence of AlgNa hydrogel and hydroxyapatite phases as well as silica bands. SEM showed the formation of specific porous relief for all types of composites. For AlgNa/2Si-BHA and AlgNa/5Si-BHA composites with different ratios of components, the skeleton density was in the range of 1.14-1.66 g/cm<sup>3</sup>. Swelling studies demonstrated a significant effect of silicon on equilibrium swelling degree, namely, it is increasing for AlgNa/Si-BHA compared to AlgNa/BHA and allows obtaining composites with swelling higher by 30 % in contrast to a pure hydrogel, which confirms the feasibility of creating this type of hydrogels. Thus, the study of the phase composition, structure, and physical and chemical properties showed the perspectives of the creation of such composite materials for medical applications.

# The use of very fast solid-state NMR spectroscopy and DFT calculations to design the microstructure of alginate chains cross-linked by paramagnetic ions

<u>Martina Urbanova</u><sup>1</sup>, Libor Kobera<sup>1</sup>, Miroslava Pavelkova<sup>2</sup>, Katerina Kubova<sup>2</sup>, Jiri Brus<sup>1</sup> <sup>1</sup>Department of NMR spectroscopy, Institute of Macromolecular Chemistry, Czech Academy of Sciences, Czech Republic <sup>2</sup>Department of Pharmaceutical Technology, Faculty of Pharmacy, Masaryk University Brno, Czech Republic

The metal ion cross-linked carbohydrates have attracted considerable interest due to their excellent properties such as self-healing, rapid recovery, biocompatibility and high mechanical properties combined with multi-stimulus responsiveness.

One of such polysaccharides is alginate (ALG), a naturally occurring biopolymer derived from brown seaweed. Its chemical structure contains  $\beta$ -D-mannuronic acid (M) and  $\alpha$ -L-guluronic acid (G), and the segmentation of the G and M residues is responsible for its properties (gelation and viscosity).

Unfortunately, the detailed structural data are entirely unavailable and completely lost if paramagnetic ions such as  $Fe^{3+}$ ,  $Mn^{2+}$  or  $Cu^{2+}$  are used as crosslinking agents. Due to the strong paramagnetic effects of these ions including extreme signal broadening and fast coherence decay the vast majority of traditional techniques of ss-NMR spectroscopy fail. These  $Fe^{3+}$ ,  $Mn^{2+}$  or  $Cu^{2+}$  ions are, however, particularly interesting and important due to their bioactive properties. In our research we have focused for obtaining the unique and up to now unreported insight into the structure of multicomponent alginate gels modified by lactic acid and cross-linked by paramagnetic ions ( $Cu^{2+}$  and  $Fe^{3+}$ ) which play a vital role in biological reactions and chemical catalysis. The lactic acid incorporated into the synthesized microparticles then acts as a pH-lowering agent, creating ideal conditions for the growth of probiotic bacteria, allowing to reach broad application potential ranging from controlled drug delivery to wound dressing scaffolds or tissue implants.

The combination of experiments by ssNMR spectroscopy and by DFT calculation demonstrated the formation of supramolecular assemblies' alginates gels crosslinked paramagnetic ions.

Acknowledgment: This work was supported by Czech Science Foundation (Grant No. GA 22-03187S).

# Structure and dynamics of multicomponent polycrystalline materials at atomic resolution

Jiri Brus, Martina Urbanova, Jiri Czernek, Jakub Obuch Department of NMR spectroscopy, Institute of Macromolecular Chemistry, Czech Academy of Sciences, Czech Republic

A growing number of currently discovered drugs may never reach their true potential. This is due to unfavorable physicochemical properties. Recent efforts to optimize their therapeutic efficacy have led to the development of multi-component drug delivery solids that perform multiple functions. However, the development of these materials is dependent on precise structural analysis at the level of atomic resolution. This is a stringent requirement as these systems straddle the boundary between crystalline and amorphous solids for which high quality diffraction data is inherently unavailable. This contribution addresses our attempt to formulate an efficient strategy for obtaining deep insight into the structure of polycrystalline composites with micro- and nanodomain architecture. This strategy is based on the combined application of domain-selective solid-state NMR spectroscopy (ss-NMR), crystal structure prediction (CSP), and density functional theory (DFT)-based calculations of NMR chemical shifts. The potential of this combined analytical approach is illustrated using the recently developed biodegradable, injectable polyanhydride microbead formulation of decitabine (5-aza-2'-deoxycytidine), an archetypal DNA methyltransferase inhibitor used as a potent therapeutic agent for epigenetic cancer therapy. The power of this approach is also demonstrated by the de novo determination of the crystal structure of the chemotactic N-formyl-L-Met-L-Leu-L-Phe-OH tripeptide, a typical model for compounds with antimicrobial activity. This study thus demonstrates the synergistic effects of the proposed combination of several experimental and computational techniques, which significantly extends the NMR crystallography approach to the field of complex mixtures and nanostructured composites and hybrid materials.

Acknowledgment: This work was supported by Czech Science Foundation (Grant No. GA 22-03187S and 23-05293S).

# Improved solubility and certain ratio of tautomeric forms of curcumin in the nanoformulations with alkylammonium dimeric surfactants

Olga Kazakova, Natalia Lipkovska, Valentyna Barvinchenko Chuiko Institute of Surface Chemistry, NAS of Ukraine, 17 General Naumov Str., Kyiv 03164, Ukraine

Curcumin is a natural hydrophobic compound with important medicinal properties that are limited due to its extremely low solubility. Colloidal delivery systems based on micelles and micellar aggregates of surfactants are commonly used to improve water solubility and bioavailability of hydrophobic molecules. In this study, we present cationic alkylammonium dimeric surfactants ethonium (CAS No. 21954-74-5) and decamethoxin (CAS No. 38146-42-8) which have the same polar hydrophilic groups, but differ significantly in the size of the spacers, the length of the hydrophobic chains, and the CMC values.

Curcumin exists in two tautomeric forms, keto and enol, which have different spectral and pharmacological properties. Significant differences were found in the effect of surfactants in premicellar concentrations on curcumin solubility and tautomeric transformations. In solutions of decamethoxin (long spacer and short chains), there is practically no shift of the keto-enol tautomerism of curcumin and no increase in its solubility. On the contrary, in premicellar solutions of ethonium (short spacer and long chains), curcumin dissolves mainly in the keto form, and its solubility generally increases 150 times.

DFT/B3LYP/6-31G(d,p) calculations with PCM solvation model showed that in an aqueous solution, the keto-curcumin exists mainly in the anti-configuration, which turns into the syn-configuration due to the formation of a stable complex with ethonium. Decamethoxin also forms stronger complexes with keto-curcumin than with enol, but their strength is significantly lower compared to curcumin-ethonium ones.

In organized micellar media of both surfactants, curcumin dissolves in the enol form, and its solubility increases by two orders of magnitude.

The results obtained can be used to create new effective drugs with high bioavailability of curcumin and controlled content of its tautomeric forms with various pharmacological activities.

# Combined antimicrobial effect of nanoparticles and medicinal plants against multidrug resistant microbes

<u>Viktoriia Holubnycha</u>, Anna Yanovska, Roman Pshenychnyi Sumy State University, Sumy, Ukraine

Antimicrobial resistance represents a major global public health concern that causes ineffectiveness of the antibiotics and rise of mortality rate due to untreatable resistant infections. Thus, the search of new treatments is at the top of humankind demands. Nanoparticles have been proven to be effective antimicrobials. On the other hand, medicinal plants have also demonstrated different mechanisms of antimicrobial action. Combining natural products with nanoparticles may be an important strategy to combat antimicrobial resistance. The aim of this study was to investigate the potential of synergistic antimicrobial action of the nanoparticles and medicinal plants.

In this work, we investigated  $Cu/CuO_2$  and ZnO nanoparticles, water and ethanolic extracts from pomegranate peel. Their individual antibacterial activity and synergistic potential of their combination were assessed against multi-drug resistant Gram-negative and Gram-positive bacteria.

The examined extracts and nanoparticles demonstrated various individual antimicrobial activity against tested multi-drug resistant microorganisms.  $Cu/CuO_2$  nanoparticles were effective against multi-drug resistant microorganisms at a lower concentration than ZnO nanoparticles. The type of solvent did not affect the antimicrobial effectiveness of the pomegranate peel. Combining plant materials with nanoparticles has led to their enhanced antimicrobial efficacy against multi-drug resistant bacteria.

Our findings reveal that pomegranate peel extract exhibits remarkable adjuvant potential to increase the effectiveness of nanoparticles against resistant bacteria. That can be used in the creation of various composite materials with improved properties.

Acknowledgment: This work was supported by the Erazmus JM project Nº 101048202 and Ministry of Education and Science of Ukraine project "Development of osteoconductive materials with improved osteoregenerative and antimicrobial potential for the restoration of bone tissue" Grant number 0124U000540.

# WRTCS Plenary Lectures

# Sintering-Assisted Additive Manufacturing

Eugen Olevsky College of Engineering, San Diego State University, USA

The specific structures of powder materials produced through additive manufacturing methods (such as binder-jetting, stereolithography, robocasting, and selective laser sintering) for complex-shaped components require careful optimization of the sintering process for porous 3D-printed products. Optimizing the additive manufacturing process for green parts enhances the final product quality by reducing shape distortions, surface roughness, and residual porosity, as well as improving the subsequent sintering steps. The sintering stage demands a thorough understanding of the high-temperature deformation behavior of the 3D-printed porous specimens. In particular, the effects of fabrication directionality and gravity on the micro- and macro-structure of sintered components remain poorly understood. Ensuring the densification of complex shapes involves controlling gravity-related and anisotropic phenomena to achieve nearly complete and distortion-free densification. Therefore, the unique features of 3D-printed microstructures necessitate the development or modification of sintering theories. The studies conducted address these challenges by involving modified sintering constitutive models, comprehensive finite element simulations, and experimental validation of the developed models. These models describe the sintering of 3D-printed objects in comparison to conventionally produced porous sintering preforms. Validation of the developed models is achieved through comparison with experimental results obtained from sintering printed powder ceramic and metallic components. The findings demonstrate how analytical engineering criteria, applicable to the design recommendations for sintered 3Dprinted parts, can be derived.

# What we understand and what we need to know in sintering

Suk-Joong L. Kang KAIST, Daejeon, Republic of Korea

Sintering is probably the oldest human technology with the firing of pottery. Yet, modern ceramic products and powder metallurgical parts are produced mostly by the sintering technique. In this respect, it would be worth to look at our past achievements and discuss the future research directions in sintering science and technology.

This presentation will first review our current understanding of sintering phenomena – densification, grain growth and microstructural evolution – during solid state sintering (SSS) and liquid phase sintering (LPS). An emphasis will be laid on a recent issue of the effects of interfacial energy anisotropy on the sintering phenomena. Future research directions in sintering science and technology will then be suggested.

#### **Reference:**

1. Bordia, R.K.; Kang, S.J.L.; Olevsky, E. Current understanding and future research directions at the onset of the next century of sintering science and technology. J. Am. Ceram. Soc. 2017, 100, 2314–2352.

# Advanced sintering methods for solid-state batteries

**Olivier Guillon** 

Institute of Energy and Climate Research: Materials Synthesis and Processing, Forschungszentrum Jülich and RWTH Aachen University, Germany

Among possible future electrochemical storage technologies, all-solid-state batteries raise high expectations in terms of energy density and safety, especially when oxide electrolytes are implemented. On the one hand, high-quality free-standing separators are required to enable high-capacity metallic anodes without catastrophic dendrite growth. On the other hand, the combination of solid electrolyte and compatible active cathode materials into thick composites cathodes with percolating pathways for both ion and electron transports is one requirement of vital importance. The quality of the interfaces is crucial to reduce the cell impedance.

In order to achieve these goals as well as to save energy and time during the processing of battery cell components, innovative sintering methods are required. In the talk, recent work on Field Assisted Sintering Technique / Spark Plasma Sintering (FAST/SPS), Cold Sintering and Ultrafast High-Temperature Sintering will be presented.

### Non-isothermal sintering of nanostructured particulate materials: Dream or reality?

Andrey V. Ragulya Frantsevich Institute of Problems in Materials Science NAS of Ukraine, 3, Omelyana Pritsaka str., 03142 Kyiv, Ukraine

Prof. Valeriy V. Skorokhod, the great scientist and philosopher of sintering, paid special attention to the influence of heating rate on the sintering of particulate bodies. He discussed a lot the development of Dr. V. Ivensen's ideas concerning activation of shrinkage in the case of rapid temperature increase. Initial lvensen's theory of non-isothermal sintering was grounded on the formal physico-chemical kinetics and treatment of numerous experimental observations just to qualify the activation energies of the shrinkage process at any density. These studies were discussed then in the framework of the rheological theory of sintering by V. Skorokhod within the large topical discussion about the role of defects of the crystal lattice on the densification activity during sintering. Leading scientists such as Profs. Ya. Geguzin, R. German, E. Olevsky, M. Harmer, Lynn-Johnson, M. Ristich, D. Uskokovich, and many others paid a lot of attention to the non-isothermal stage of sintering and its theoretical justifications using discrete and continual models. Thus, Prof. R. German has modified the model systems of G. Kuczynski's equations for the non-isothermal case. Prof. Lynn-Johnson has proposed the "Master Sintering Curve" method for the analysis of the non-isothermal stage and predicting the best heating regime. Prof. E. Olevsky has developed a continual theory of sintering for the non-isothermal case. Prof. M. Harmer hypothesized a rapid overcoming of the temperature range, where the coalescent growth of grains is dominating over shrinkage and proved its validity experimentally. Prof. H. Palmour III, who proposed a method of rate-controlled sintering, has also grounded on Harmer's hypothesis, and for the first time put the heating rate as a function of the shrinkage rate. In most of the listed works, the kinetic analyses of sintering were limited to the changes in such macroparameters as shrinkage and porosity without reference to the real structure, primarily the porous and grain structure and their interrelated evolution. Perhaps, H. Palmour III has examined in detail the limitations of the shrinkage rate in relation to the changing morphology of open and closed pores in all porosity ranges.

Ultrafine and nano-sized powders have stimulated further studies of non-isothermal stage of sintering as it turned out that almost 100 % densification occurs during heating only under non-linear mode.All the above achievements preceded the rapid development of modern methods of sintering under the influence of external mechanical, electrical, magnetic, electromagnetic fields: induction, spark-plasma, microwave, laser and flash sintering, in which the duration of sintering was reduced to tens of seconds or minutes. This rapid development is in progress for now, which ensures the creation of the latest materials and competitive technologies in the world. For all these methods, the operating parameters have been established to achieve full density and nanosized grains after sintering for the sake of significantly improved properties of materials due to the size effect.

# Spark plasma sintering of thermoelectric materials

Jing-Feng Li

# School of Materials Science and Engineering, Tsinghua University, Beijing, China

Thermoelectric technology that are capable of direct interconversion between heat and electricity have drawn increasing attention both from scientific and industrial interests, so the development of high-performance thermoelectric materials has been one of the frontier fields of functional materials research. In the last decades, great progress has been made in thermoelectricity research, and material processing has made important contributions to thermoelectricity research. Spark plasma sintering (SPS) is increasingly used for processing thermoelectric materials, as a rapid sintering process with advantages of lower sintering temperature and short holding times for synthesizing fine-grained microstructures, which are usually required for developing thermoelectric materials with high dimensionless figure of merit (ZT) benefiting from a reduced thermal conductivity. Also importantly, most thermoelectric materials must be sintered in a reduced atmosphere, which can be easily realized in SPS. Bi<sub>2</sub>Te<sub>3</sub> alloys as representative thermoelectric materials are conventionally fabricated by the zone-melting method, but their ZT values remain lower than unity. Substantial increase in ZT values has been achieved in the SPS-processed Bi<sub>2</sub>Te<sub>3</sub>-based materials. GeTe and Mg<sub>3</sub>(Sb,Bi)<sub>2</sub> are new thermoelectric materials with high ZT at middle temperatures. It was found that increasing electrical conductivity and reducing thermal conductivity can be achieved simultaneously by suitably increasing SPS temperature, leading to a significant ZT enhancement in both materials. By focusing on three representative examples, this talk will show how SPS is effectively employed for developing high-performance thermoelectric materials.

# Flash sintering of carbides and borides

<u>Vincenzo M. Sglavo</u>, Emanuele De Bona, Isacco Mazo Department of Industrial Engineering, University of Trento, Trento, Italy

Flash sintering was officially discovered about fifteen years ago as a ground-breaking method to consolidate ceramics in a very short time at temperature much lower than that used for conventional sintering. Since then, it has been applied to several ceramics and composites with the common feature to be characterized by a negative temperature coefficient (NTC) for resistivity while few attempts have been made on materials with metal-like electronic conduction like hard ceramics, i.e. borides and carbides.

WC, ZrB<sub>2</sub> and ZrC commercial powders were used in the present work. Flash sintering experiments were carried out using a custom-made apparatus operating in lab air, which allowed to control the applied pressure and voltage, temperature and displacement. The obtained materials were characterized from a physical, structural and mechanical point of view. Tungsten carbide, zirconium diboride (and their composites) and zirconium carbide can be successfully flash sintered by using optimized processing conditions in very short time (less than a minute). Final microstructure, density and mechanical properties (like hardness and fracture toughness) depend on three fundamental processing parameters like surface chemistry of the starting powder, applied pressure and voltage.

Sintering behaviour is correlated with a thermal runaway phenomenon generated by the extrinsic NTC behaviour of the powder compact at the beginning of the process although the considered materials are intrinsically PTC (positive temperature coefficient for resistivity) like metals. Surface chemistry of the starting powder and pressure have a fundamental role in the densification behaviour since they determine the initial electrical resistance of the powder compact and, therefore, influence the power which is initially dissipated in the material to activate the diffusional phenomena necessary for sintering.

The results of the present work greatly expand the potentiality of flash sintering as an efficient, low-energy intensity process for electrically conductive materials and, especially, hard ceramics.

# Synthesis and sintering of sulfide-based optical ceramics

Yiquan Wu

Kazuo Inamori School of Engineering, New York State College of Ceramics, Alfred University, Alfred, New York 14802, United States

Due to their favorable optical performance and mechanical properties, zinc sulfide (ZnS) and calcium lanthanum sulfide ( $CaLa_2S_4$ ) have been studied as promising candidates for infrared optical ceramics. In this work, ZnS and  $CaLa_2S_4$  powders were first synthesized by using a wet chemistry method to form a ceramic powder and then were sintered at different temperatures by using a hot-pressure and a field-assisted sintering technique to process bulk ceramics. Through a colloidal processing method, ZnS powder with homogeneous morphology and large surface area was synthesized and  $CaLa_2S_4$  precursor was synthesized by using a facile ethanolbased single-source precursor route. The effects of varying different processing parameters, in both the powder synthesis and consolidation stages, were studied to develop a procedure for fabricating sulfide-based optical ceramics. Sintering behaviors and grain growth kinetics were studied through densification curves and microstructural characterizations, from which the diffusion mechanisms to control grain growth were analyzed. The phase compositions and morphologies of the synthesized powder and sintered ceramics were studied by using X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM), respectively, in addition to the surface area and pore size analyses and optical characterization.

### **Powder-Free Processing of Advanced Ceramics with Multifunctional Properties**

Ralf Riedel

Institute of Materials Science, Darmstadt University of Technology, Otto-Berndt-Str.3, D- 64287 Darmstadt, Germany

There is presently much effort in basic science and applied research to work on novel materials with properties far beyond that of the existing ones. The aim and scope of the research in this field is to develop materials with superior thermomechanical, physical and chemical properties. In particular, the synthesis of carbonitride and oxycarbide based ceramic devices from molecular inorganic polymers has attracted increasing attention to produce dense and porous ceramic composites, fibers or coatings. One important advantage of polymer derived ceramics is their potentially simple processing to complex components by extrusion or injection molding of polymer masses or by cold machining of compacted polymer parts. These processing routes avoid the use of ceramic starting powders and can be considered as powder-free technology. Moreover, novel ceramic compositions such as ternary, guaternary and guinary silicon based carbonitrides and oxycarbides can be synthesized by the polymer-to-ceramic transformation route. While silicon containing carbonitrides have been found to be extremely high temperature resistant with respect to crystallization, decomposition, creep, and oxidation, silicon based oxycarbides reveal a similar property profile with lower values but at a significant lower cost level. In this presentation, the progress in synthesis and processing of molecular preceramic compounds as well as some properties of advanced ceramics and ceramic nanocomposites derived therefrom are reviewed.

#### **Reference:**

1. P. Colombo, G. Mera, R. Riedel. G.D. Soraru, *J. Am. Ceram. Soc.* (2010) https://doi.org/10.1111/j.1551-2916.2010.03876.x

#### W.PL.S.II.9

# Optimizing the performance of metastable beta titanium alloys through processing (*e.g.* additive manufacturing) and heat-treatment

Hamish L Fraser

Center for the Accelerated Maturation of Materials, Dept. of Materials Science and Engineering, The Ohio State University, Columbus, OH, USA

Metastable beta titanium alloys offer a range of attractive properties for structural applications. This paper provides an understanding of the origin of these properties, focusing on the differences between metastable beta and alpha/beta alloys. Of course, it is important to realize optimum properties in processed materials, and in this talk, we focus on Additive Manufacturing (AM) of components, with a focus on realizing optimum properties. In the case of titanium alloy components, the application of essentially all industrially competitive techniques for additive manufacturing result in characteristic defects, being coarse columnar grains (in the direction of deposition), porosity, and residual stresses. In this paper, ways of avoiding coarse columnar grains has been addressed. The proposed solution involved the application of computational thermodynamics to identify which alloying additions to titanium alloys result in an increase in the freezing range of the given alloy base, such that a columnar to equiaxed transition (CET) may be effected. These alloying additions, mainly eutectoid formers, have been found at critical concentrations, to cause a CET to occur, resulting in a relatively fine equiaxed microstructure. While the refined microstructure is attractive, there are consequences associated with this alloying approach, involving the precipitation of intermetallics during subsequent heat-treatments, and a change in the character of the specific titanium alloys. It will be shown that a very attractive metastable beta alloy results as a result of this alloying approach, and the properties of this alloy will be presented and discussed.

# WRTCS Oral Presentations

#### Fabrication of High Entropy Alloys and Carbides via spark plasma sintering

Daniel Valášek<sup>1</sup>, David Salamon<sup>1,2</sup> <sup>1</sup>Department of Advanced Ceramic Materials, CEITEC Brno University of Technology, Purkyňova 123, Brno, Czech Republic <sup>2</sup>Department of Materials Science, Montanuniversitat Leoben, Franz Josef-Strasse 18, A-8700, Leoben, Austria

High entropy alloys (HEA) are a class of advanced materials discovered in 2004. These alloys are defined as multicomponent materials containing at least five different elements in equimolar or near equimolar ratios and having a mixing entropy greater than 1.5*R*. These alloys have been proven to have superior properties, such as higher strength and corrosion resistance, compared to conventional alloys. The discovery of HEA was followed by the discovery of High Entropy Ceramics (HECer), which include an additional non-metallic element in their crystal structure. Various groups of HECer and their properties differ based on this non-metallic element (for example, O, B, N, and C), offering a wide range of new materials with superior properties. High Entropy Carbides (HEC), for example, offer increased hardness and oxidation resistance compared to conventional carbides.

Several sintering techniques have been tested over the years to prepare both HEA and HECer, but Spark Plasma Sintering (SPS) remains the dominant production method used for HECer, and it is also possible to use it to prepare HEA.

In the presented work, a novel preparation route has been used to prepare high entropy carbides. This route involves using HEA as the starting material for preparing HEC by reactive sintering in the SPS. This route allows the modification of the carbon added to the starting alloy and is less susceptible to oxidation than previously reported routes. The described approach has been used to prepare HEC, which consists of niobium, molybdenum, tantalum, tungsten, and vanadium. In addition, other carbides with unique microstructures were prepared. The presented work also includes results from optimizing the preparation route consisting of milling and sintering the starting mixture in the SPS at various temperatures from 1800 °C to 2100 °C with the applied pressure of 50 MPa. Sintered carbides and alloys were further characterized using scanning electron microscopy, energy-dispersive X-ray spectroscopy, and X-ray diffraction. The mechanical properties of the sintered materials were examined using Vickers hardness measurement and nanoindentation.

## Bulk Ti and Ti6Al4V through Consolidation of Chips by Severe Plastic Deformation Methods

<u>Peter Cengeri</u><sup>2</sup>, Jelena Horky<sup>1</sup>, Laszlo Sajti<sup>1</sup>, Michael J. Zehetbauer<sup>2</sup>, Bartosz Sulkowski<sup>3</sup>, Grzegorz Boczkal<sup>3</sup>, Erhard Schafler<sup>2</sup> <sup>1</sup>RHP-Technology GmbH, Seibersdorf, Austria <sup>2</sup>Faculty of Physics, University of Vienna, Wien, Austria <sup>3</sup>Department of Materials Science & Non-Ferrous Metals Engineering, Faculty of Non-Ferrous Metals, AGH University of Cracov, Krakow, Poland

Titanium is often used for highly complex, lightweight components especially in aviation and medical applications. Its production is particularly energy-intensive due to the high oxidation tendency, and it is six times more expensive than that of steel. The machining of Titanium yields large amounts of waste in the form of chips. Conventional recycling by remelting the chips requires a lot of energy. It can be saved to a large extent by application of SPD (Severe Plastic Deformation) which uses Ti chips as starting raw material.

In the present work, the two most important Severe Plastic Deformation (SPD) methods - Equal Channel Angular Pressing (ECAP) and High Pressure Torsion (HPT) - were used for recycling and/or upcycling of titanium chips. For successful consolidation, efficient cleaning of the chips was crucial. To quantify the quality of the consolidation process, results of mechanical testing, texture analysis, and of optical and electron microscopy were compared with those from the bulk counterparts. Especially by measuring the torque characteristics during HPT deformation of the chips, the success of consolidation can be well demonstrated when comparing it with the torque characteristics of bulk samples.

It is concluded that full consolidation *i.e.* the recycling of chips using SPD is possible at temperatures which not only are significantly lower than those of melting but also than those of sintering. However, chips must be prevented from mutual sliding as plastic deformation is essential for successful consolidation. Still, the enhancement of pressure and temperature remain advantageous for consolidation.

## Thermal stress analysis on thinning and new structure of Cu Clips attached with Ag sintered layers for high performance SiC chip systems

<u>Daito Murakami</u><sup>1</sup>, Masaaki Aoki<sup>1,2</sup>, Kazuma Yamashita<sup>1</sup>, Maurizio Fenech<sup>3</sup>, Riski Wirawan<sup>3</sup>, Nobuhiko Nakano<sup>1</sup>

<sup>1</sup>Department of Electronics and Electrical Engineering, Faculty of Science and Technology, Keio University, Yokohama, Kanagawa 223-8521, Japan

<sup>2</sup>MacDermid Alpha Electronics Solution /MacDermid Performance Solutions Japan <sup>3</sup>Semiconductor Assembly Solutions/MacDermid Alpha Electronics Solutions

SiC power chip systems having Cu Clip structures have been very important to offer superior heat dissipation and lower wiring resistance compared to conventional bonding wires. Ag sintering attachment of Cu Clip on SiC chip can realize highly efficient heat dissipation. Ag sintered layer (SL) has high melting point, high thermal conductivity, and low resistance. However, these SiC systems have not yet undergone sufficient reliability evaluation.

In this research we conducted structural modeling and evaluation of reliability through thinning of Cu Clip to assess the reliability of Clip structures on chips. We also evaluated new shapes which are strip-shape and multi-perforated structure of Clip corresponding to a Clip bonding on chips. Stress and deformation analysis of Clip structures was performed by 3D multi-physics solver, and Clip-bonding reliability was simulated. As a criterion for reliability evaluation, we analyzed von Mises stresses and normal stresses in vertical and horizontal directions in Ag SLs on chips and clip structure. Deformation of chip system was also analyzed. The target chip system consisted of a 7mm x 7mm SiC chip mounted on Active Metal Brazing (AMB) substrate with Si<sub>3</sub>N<sub>4</sub> film using Ag SL, and a Cu Clip attached by Ag SL on a chip. In the absence of Cu Clip the upward bending occurs at the chip area due to stronger thermal contraction in lower Cu of AMB. It was found that this bending is alleviated when Cu Clips are attached. We compared thermal stress distributions in Ag SL for Cu Clip thicknesses ranging from 100 to 400 micrometers. Thinner Cu Clips resulted in larger bending at the chip area, and lower perpendicular tensile stresses at the edges of Ag SLs in both chip and substrate areas. Additionally, changing the shape of the Clip on the chip resulted in a similar effect to reducing Clip thickness. These findings suggest that the design of Clip thickness and shape are very essential for high-performance and reliable Ag sintering Clip-attachment. Our analytical approach and results are highly useful for the design of reliable SiC power chips with Ag SLs.

## Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXenes surface exploitation for the practical applications

<u>Simonas Ramanavicius</u><sup>1</sup>, Anton Popov<sup>2</sup>, Sarunas Zukauskas<sup>3</sup>, Sonata Adomaviciūtė-Grabusove<sup>4</sup>, Martynas Talaikis<sup>1</sup>, Valdas Sablinskas<sup>4</sup>, Oleksiy Gogotsi<sup>5</sup>, Yury Gogotsi<sup>6</sup>, Gediminas Niaura<sup>1</sup>, Almira Ramanaviciene<sup>2</sup>, Arunas Ramanavicius<sup>3</sup>
 <sup>1</sup>State Research Institute Center for Physical Sciences and Technology (FTMC), Sauletekio av. 3, LT-10257 Vilnius, Lithuania
 <sup>2</sup>NanoTechnas—Center of Nanotechnology and Materials Science, Faculty of Chemistry and Geosciences, Vilnius University, Naugarduko St. 24, LT-03225 Vilnius, Lithuania
 <sup>3</sup>Department of Physical Chemistry, Faculty of Chemistry and Geosciences, Institute of Chemistry, Vilnius University, Naugarduko 24, LT-03225 Vilnius, Lithuania
 <sup>4</sup>Institute of Chemical Physics, Vilnius University, Sauletekio Av. 3, LT-10257 Vilnius
 <sup>5</sup>Materials Research Center Ltd., Krzhyzhanovskogo Str. 3, 01001 Kiev, Ukraine
 <sup>6</sup>Department of Materials Science and Engineering and A.J. Drexel Nanomaterials Institute, Drexel University, Philadelphia, PA, USA

 $Ti_3C_2T_x$  is the first discovered and the most intensely studied MXenes with many unique and favorable properties [1]. One such property is complex and controllable surface chemistry, which leads to the application in adsorbing and sensing of various molecules [2,3]. However, no matter the studies published on applications based on the surfaces, many challenges exist to overcome for broader MXenes applications. This study focuses on how tunable and versatile MXenes are for applications based on surface chemistry, such as sensors and adsorbents. It was revealed that MXenes are applicable to the adsorption and sensing of molecules by different methods. In some cases, significant selectivity towards target analytes was noticed, and trends for favorable sensor design for target analytes were revealed. The collected data is expected to impact the development of MXenes-based sensors and their practical application.

## **References:**

- 1. Naguib, M.; Kurtoglu, M.; Presser, V.; Lu, J.; Niu, J.; Heon, M.; Hultman, L.; Gogotsi, Y.; Barsoum, M.W. Two-dimensional nanocrystals produced by exfoliation of Ti3 AlC2. *Adv Mater*. **2011**, *23*, 4248–4253.
- 2. Ramanavicius, S.; Ramanavicius, A. Progress and Insights in the Application of MXenes as New 2D Nano-Materials Suitable for Biosensors and Biofuel Cell Design. *Int. J. Mol. Sci.* **2020**, *21*, 9224.
- Adomavičiūtė-Grabusovė, S.; Ramanavičius, S.; Popov, A.; Šablinskas, V.; Gogotsi, O.; Ramanavičius, A. Selective Enhancement of SERS Spectral Bands of Salicylic Acid Adsorbate on 2D Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>-Based MXene Film. *Chemosensors* **2021**, *9*, 223.

## Investigation of a UO<sub>2</sub> ceramic as a reference for a homogeneous MOX fuel

<u>Kaythleen Torrente</u><sup>1,2</sup>, Christelle Duguay<sup>2</sup>, Franck Doreau<sup>1</sup>, Guillaume Bernard-Granger<sup>1</sup> <sup>1</sup>CEA, DES, ISEC, DMRC, Univ. Montpellier, Marcoule, France <sup>2</sup>CEA, DES, IRESNE, DEC, Cadarache, France

France aims at closing its nuclear fuel cycle by recycling the valuable materials contained in the spent fuel. The most developed next generation reactor design is the Sodium Fast Reactor, the concept retained for the Phénix and Superphénix reactors in the past [1]. For their operation, these reactors use MOX fuel pellets (mixed oxides of uranium (U) and plutonium (Pu)). These small fuel cylinders, with typical diameter and height, are manufactured by a powder metallurgy route, using the COCA process (CObroyage CAdarache). During sintering several phenomena occur simultaneously. So, his work is dedicated to the investigation of these phenomena and more precisely to the fine study of the grain growth and densification mechanisms of a homogeneous MOX composition, at the scale of the spatial distribution of the U and Pu chemical elements, for different Pu contents (from 0 to 26 mol.%).

The first part of this paper will present the results obtained for the  $UO_2$  reference samples (without Pu). The second part will be devoted to the presentation of the first results in  $UPuO_{2\pm x}$  with 11 mol.% in Pu/(U+Pu).

All these tests led to the production of numerous graphs, such as densification rate (s<sup>-1</sup> or K<sup>-1</sup>) as a function of density evolution or sintering temperature. Density and grain size parameters were also measured. Ultimately, this enabled the construction of a sintering map for all three atmospheres involved. All the dilatometric curves were also processed to determine activation energies using the Master Sintering Curve (MSC) and Constant Rate of Heating (CRH) methods. The values obtained will be compared with those proposed in the literature and the limiting diffusional mechanisms identified will be presented.

### **References:**

- 1. Available online: <u>https://www.cea.fr/multimedia/Documents/publications/rapport-gestion-durable-matieres-nucleaires/Tome%203.pdf</u>
- Kato, M.; Maeda, S.; Abe, T.; Asakura, K. Uranium Oxide and MOX Production. In *Comprehensive Nuclear Materials*; Elsevier: Amsterdam, The Netherlands, 2020; Volume 2, pp. 1–34. https://doi.org/10.1016/B978-0-12-803581-8.11701-1

## Preparation of single-phase high entropy ceramic for further modification: Comparison of different sintering processes

<u>Marek Rotter</u><sup>1</sup>, Katarína Drdlíková<sup>2</sup>, Karel Maca<sup>1,2</sup> <sup>1</sup>CEITEC, Brno University of Technology, Brno, Czech Republic <sup>2</sup>Faculty of Mechanical Engineering, Brno University of Technology, Technicka 2, Brno, Czech Republic

High entropy ceramics (HECs) are single-phase materials containing five or more types of cations or anions. This provides them with enhanced properties, such as thermal and chemical stability, wear resistance and mechanical properties, compared to binary ceramics. Moreover, they usually act as semiconductors or insulators, making them more useful as functional materials. Also, HECs can be modified and prepared as transparent or/and with luminescent properties. The advantages of transparent polycrystalline ceramics are better mechanical and resistance behaviour, and they can be prepared easily, with more complex shapes than single crystals.

Polycrystalline ceramics can be transparent if no impurities are incorporated into the microstructure, together with high density (> 99.9 %). Therefore, a single-phase structure is preferred because of the suppression of the scattering mechanism due to different refractive indexes of different phases.

Due to the difficulty of meeting the above requirements, only a few transparent HECs have been produced to date. Moreover, the first attempts achieved poor transparency and most of them were prepared by conventional pressureless sintering methods. Therefore, this work aims for the successful preparation of single-phase luminescent material, which can be further modified into transparent polycrystalline ceramics.

The  $RE_2Zr_2O_7$  composition (RE stands for five different rare earth elements and yttrium) was selected because it can exist in two cubic phases, namely pyrochlore and defect-fluorite. The selection rules of elements consider the luminescent properties and ion size usable for phase prediction. The sintering was done by pressureless sintering with hot isostatic pressing and electric current-assisted sintering. The samples were evaluated in terms of final sample density obtained by the Archimedes method, microstructure and its homogeneity evaluated by SEM and XRD analysis, and luminescent properties.

*Acknowledgement:* This work has received funding from the Horizon Europe project GlaCerHub under grant agreement No. 101087154.

## Thermal stress and deformation in SiC semiconductor chip systems having three-layer stacked Clips attached by Ag sintered layers

<u>Masaaki Aoki</u><sup>1,2</sup>, Kazuma Yamashita<sup>1</sup>, Maurizio Fenech<sup>3</sup>, Riski Wirawan<sup>3</sup>, Nobuhiko Nakano<sup>1</sup>

<sup>1</sup>Department of Electronics and Electrical Engineering, Faculty of Science and Technology, Keio University, Yokohama, Kanagawa 223-8521, Japan

<sup>2</sup>MacDermid Alpha Electronics Solutions/MacDermid Performance Solutions Japan <sup>3</sup>Semiconductor Assembly Solutions/MacDermid Alpha Electronics Solutions

SiC power chip systems with metal Clips have been very important because of Clip advantages which are more efficient heat dissipation and lower electrical loss as compared to conventional bonding wires. Ag sintering Clip-attachment can increase the Clip advantages because Ag sintered bonding layer has the high thermal conductivity of about 250 W/mK and the thickness much thinner than conventional lead-free solders. Present important subject is to certify the Ag sintering Clip-attachment for SiC chip systems.

This paper presents Ag sintering attachment of the new Clips consisting of Cu/CuMo/Cu stacked layers. We demonstrate the reliability improvement of sintered layers under these new Clips by thermal stress and deformation analysis using 3D multi-physics solver based on FEM. We performed analysis and simulations at fixed ambient temperature (25 degrees Celsius) assuming the elastic stress-strain relationship.

The target SiC chip system has a SiC chip with the thickness of 150  $\mu$ m (7x7 square millimeter) attached on AMB (Active Metal Brazing) substrate with Si<sub>3</sub>N<sub>4</sub> film by Ag sintered layer (SL), and a 400  $\mu$ m thick Clip consisting of Cu/CuMo/Cu stacked layers. This 3-layer stacked Clip is also attached by Ag SL on a chip. Simulation results show that the new 3-layer stacked Clips can relax the deformation of chip systems and reduce von Mises stresses in Ag sintered bonding layers as compared to 400  $\mu$ m thick Cu Clips. It was found that the maximum normal stress at perpendicular direction inside Ag SL is tensile and appears at the Ag SL edge under Clip edge on chip. The maximum perpendicular tensile stress under the new Clip decreased to 410 MPa from the value under Cu Clip, which is 1050 MPa. The tensile stress at the Ag SL edge near Clip bridge on chip also decreased by the new Clip. These stress reductions are thought to be caused by lower Thermal Expansion Coefficient (TEC) of CuMo than Cu, which is 7.7. Thermal contraction of Cu/CuMo/Cu stacked Clip and TEC mismatch between this new Clip and SiC are smaller than Cu Clip, resulting in stress reduction within Ag SL. In conclusion the new 3-layer stacked Clips are very valuable for reliable Ag sintering Clip-attachment.

#### Success and failure of in-situ microstructure observations in metastable $\beta$ Ti alloys

Frank Niessen<sup>1,2</sup>, Ryan Naseri<sup>1</sup>, Azdiar A. Gazder<sup>1</sup>, Dmytro Savvakin<sup>3</sup>, <u>Elena Pereloma<sup>1,4</sup></u> <sup>1</sup>UOW Electron Microscopy Centre, University of Wollongong, Wollongong, NSW, Australia <sup>2</sup>Section of Materials and Surface Engineering, Department of Civil and Mechanical Engineering, Technical University of Denmark, Kongens Lyngby, Denmark

<sup>3</sup>Institute for Metal Physics, National Academy of Sciences of Ukraine, UA-03142, Kyiv, Ukraine <sup>4</sup>School of Mechanical, Materials, Mechatronic and Biomedical Engineering, University of Wollongong, NSW, Australia

Advances in in-situ techniques made it possible to shed light on the sequence of events taking place in materials under various externally imposed conditions, such as heating, cooling, or loading. Careful selection of suitable phenomena to investigate, combined with the appropriate choice of in-situ technique forms the basis for the successful outcome of an experiment.

In this presentation, examples of both in-situ transmission electron microscopy (TEM) and scanning electron microscopy (SEM) combined with electron back-scattering diffraction (EBSD) and energy dispersive X-ray spectroscopy (EDS) are provided. These include:

In-situ TEM study of tensile deformation of a metastable  $\beta$  Ti-10V-2Fe-3Al (wt.%) alloy highlighted the need for correct sample selection and the difficulty in initiating the deformation-induced  $\alpha''$  martensite transformation in these miniature samples. While no martensite formation was detected in samples comprising only  $\beta$  phase, it was initiated when a  $\beta/\alpha$  interface was present. The former was linked to the easy escape of dislocations at the surface preventing strain accumulation and nucleation of martensite in  $\beta$  phase.

In-situ SEM investigation of bending behavior in a metastable  $\beta$  Ti wrought and produced by blended elemental powder metallurgy (BEPM) Ti-10V-2Fe-3Al (wt.%) alloys was carried out. The simultaneous EBSD and EDS data acquisition at selected loads revealed the initiation, growth, variant selection and interactions of orthorhombic  $\alpha$ " martensite plates in a body-centred cubic  $\beta$  matrix of wrought alloy. Contrarily, no deformation-induced  $\alpha$ "martensite formation was detected in BEMP Ti alloy until nearly fractured due to the load-bearing capacity of the constituent voids. Only in 1-2  $\beta$  grain layers near fracture, {332}(113)<sub> $\beta$ </sub> deformation twins and deformation-induced  $\alpha$ " and  $\omega$  phases formed.

# Reactive sintering behavior and enhanced densification of diboride-carbide composites

Sijia Huo, Yujin Wang, Lei Chen, Yu Zhou

School of Material Science and Engineering, Harbin Institute of Technology, Harbin 150001, China

Ultrahigh-temperature ceramics (UHTCs), including diborides and carbides of transition metals, exhibit excellent mechanical properties, good heat and chemical resistance, and unusually good electrical and thermal conductivities, which makes them a class of materials with potential applications in extreme environments. However, it is usually difficult to achieve densification due to the high melting point, strong covalent bond and low self-diffusion coefficient of UHTCs. Fortunately, some diborides and carbides can undergo chemical reactions to exchange anions and cations and form solid solutions at the same time. Compared to single-phase self-diffusion, this novel solid solution & reaction coupling driven inter-diffusion process can enhance mass transfer, promote material densification, and introduce additional solid solution phases. The formation of multiple solid solutions and microstructure refinement introduced by reaction sintering typically improve the mechanical properties of the materials. This work provides new ideas for the optimization, design, strengthening, and toughening of carbide-diboride composite ceramics.

O.S.II.W.10

## **Entropy as an Order Parameter in Thermodynamics**

Yuri Kornyushin

#### Maître Jean Brunschvig Research Unit, 59/39 King George Street, Jerusalem 94261, Israel

Rudolf Clausius had introduced Entropy as a measure of order/disorder (that is as an Order Parameter) in the early 1850<sup>th</sup>.

In 1937 Lev Landau introduced another order parameter also. The order parameter of Landau is different in every specific case. It should be determined for every specific case independently. Entropy is a universal parameter, all the same for every specific case. This is a great advantage. The author started to use Entropy as an order parameter in the early 1980<sup>th</sup>.

This technique allowed the author to formulate a general formulation of Thermodynamics of Metastable States [1].

The general theory was reported as a key lecture on the 13<sup>th</sup> Colloquium on Thermophysical Properties in Boulder, Colorado, USA, and it is available free for everybody on The Net Advance of Physics site of MIT in Metastability topic.

#### **Reference:**

1. Kornyushin, Y. Phenomenological Thermodynamics of Metastable States. J. Non-Equilib. Thermodyn. 2000, 25, 15–30.

# WRTCS Poster Presentations

## Synthesis and characterization of In-doped BaSnO<sub>3</sub> electrolyte for intermediatetemperature solid oxide fuel cells

<u>Jelena Mitrović</u><sup>1</sup>, Milica Počuča-Nešić<sup>1</sup>, Matejka Podlogar<sup>2</sup>, Aleksandar Malešević<sup>1</sup>, Aleksandar Radojković<sup>1</sup>, Olivera Zemljak<sup>1</sup>, Katarina Vojisavljević<sup>1</sup>, Zorica Branković<sup>1</sup>, Goran Branković<sup>1</sup>

<sup>1</sup>University of Belgrade, Institute for Multidisciplinary Research, Belgrade, Serbia <sup>2</sup>Jožef Stefan Institute, Department for Nanostructured Materials, Ljubljana Slovenia

 $BaSnO_3$  is a good candidate for intermediate-temperature solid oxide fuel cell (IT-SOFC) electrolyte material because of its high proton conductivity, ideal cubic crystal lattice, stable phase composition up to 1000 °C, good thermal and chemical stability in different atmospheres, easy preparation methods and non-toxicity. Its proton conductivity can be significantly improved by doping with In on Sn-site in the BSO crystal lattice.

The aim of this work is to investigate the cold sintering, a relatively new low-temperature sintering technique, for the preparation of dense indium doped BaSnO<sub>3</sub> electrolyte with the composition BaSn<sub>1-x</sub>In<sub>x</sub>O<sub>3</sub>, BSIO (x = 0.00, 0.10, 0.15 and 0.20). This sintering technique enables full densification and controlled microstructure design of ceramic materials at low temperatures (<300 °C) within short duration (~1 h).

BSIO powders were prepared by polymerization method and subsequently cold sintered at 250 °C for 30 min and 1 h using different types and amount of the liquid phase. The structural properties of BSIO sintered samples were examined by XRD analysis, while the FESEM, TEM and HRTEM analyses were used for their microstructural properties. Total electrical conductivity of dense BSIO-based electrolyte was investigated by impedance spectroscopy in the temperature range of 400 to 700 °C in a wet hydrogen atmosphere.

**Acknowledgement**: This research was supported by JECS trust (the visit of 8<sup>th</sup> May to 5<sup>th</sup> August at Jožef Stefan Institute, Ljubljana, Slovenia, Contract No: 2024 398).

#### Comparison of TiCN-based cermets sintered under different atmospheres

<u>René M. Guillen Pineda</u>, Hortensia Melero, Olivier Ther Hyperion Materials & Technologies Spain, S.L.

Cermets are an advanced composite material that mix a hard ceramic phase along with a metallic binder (Figure 1). Cermets are a special kind of composite material that provides high performance, including high mechanical characteristics and wear resistance. Titanium carbonitride is one of the basic raw materials used to fabricate cermet materials. The typical microstructure of Ti (C, N)-based cermets consists of a core-rim grain structure or Ti (C, N) particles bonded with a metallic binder. The typical core-rim structure is formed through the dissolution and precipitation process. Figure 2 shows the core-rim grain structure can be divided into three zones: the core, the inner rim, and the outer rim. Based on the chemical composition, grain size, and sintering schedule, two types of core-rim structures can be observed: a black core with white. The cermets present promising and different properties as good thermal shock and oxidation resistance. It has been widely used in cutting cast iron, hard alloy milling cutter, milling cutter, knife, and plane blade. One of the most important properties of these materials is sintering at low temperatures associated with small grain size in the sintered products. A deeper look at the effect of the C and N ratio (30-70, 50-50, and 70-30) initially present in the TiCN raw material highlighted a surprising behavior. Figure 3 displays the interaction and results of the mechanical properties of different raw materials and the atmospheres. In these materials hardness is decreasing with the increase of N content, even though N is a well-known grain growth inhibitor for Ti hard phase. By another hand, the selection of a proper sintering atmosphere (Vacuum, Vacuum +  $N_2$ ) will corroborate which raw material is suitable to develop new Cermet composition with optimal final properties.

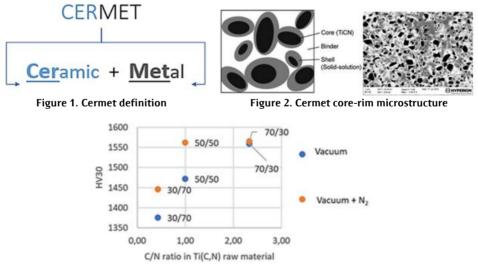


Figure 3. Mechanical properties of TiCN raw materials sintered in different atmosferes

## Structural, microstructural and multiferroic properties of YMnO<sub>3</sub> ceramics co-doped with titanium and rare-earth metals

<u>Olivera Zemljak</u><sup>1</sup>, Danijela Luković Golić<sup>1</sup>, Bojana Simović<sup>1</sup>, Pavla Šenjug<sup>2</sup>, Damir Pajić<sup>2</sup>, Matejka Podlogar<sup>3</sup>, Aleksandar Malešević<sup>1</sup>, Jelena Mitrović<sup>1</sup>, Goran Branković<sup>1</sup>, Zorica Branković<sup>1</sup>

<sup>1</sup>Institute for Multidisciplinary Research, University of Belgrade, Belgrade, Serbia <sup>2</sup>Department of Physics, Faculty of Science, University of Zagreb, Zagreb, Croatia <sup>3</sup>Department for Nanostructural Materials, Jožef Stefan Institute, Ljubljana, Slovenia

Hexagonal manganites, RMnO<sub>3</sub> (R- rare-earth element or yttrium), are multiferroic materials with ferroelectric and antiferromagnetic ordering, that open the possibility of coupling between them i.e. the opportunity of switching magnetization by an electric field and/or electric polarization by a magnetic field. Hexagonal  $YMnO_3$  is the most commonly investigated hexagonal manganite, with a high ferroelectric Curie temperature ( $T_c \approx 900$  K) and a low Néel temperature ( $T_{\rm N} \approx 75$  K). At room temperature, it exhibits a non-centrosymmetric structure with space group  $P6_{3}cm$ . Microcracking and porosity observed in YMnO<sub>3</sub> ceramics limit application possibilities. The presented results indicated the influence of partial substitution of  $Y^{3+}$  with La<sup>3+</sup>, Gd<sup>3+</sup>, Er<sup>3+</sup> and Yb<sup>3+</sup>, and Mn<sup>3+</sup> with Ti<sup>4+</sup>, on the properties of YMnO<sub>3</sub> ceramics. The  $Y_{1-x}R_xMn_{0.90}Ti_{0.10}O_{3+\delta}$  (*R* = La; Gd; Er; Yb and *x* = 0.005; 0.01; 0.02; 0.05) powders were synthesized using the sol-gel, polymerization complex method from citrate precursors, and then calcinated at 900 °C for 4 h. The ceramic samples were obtained after sintering at 1380, 1400 or 1420 °C for 2 h, depending on the type of dopant and its concentration. All doped samples crystallized in rhombohedral  $1 \times 1 \times 3$  superstructure with R3c space group, without the presence of secondary phases. The morphology of the samples revealed non-uniform grain shapes and wide ranges of grain sizes, with a mostly low concentration of microcracks and inter- and intragranular pores. The ferroelectric response of doped samples did not significantly improve relative to  $YMn_{0.90}Ti_{0.10}O_{3+6}$ , but they showed a reduction of the leakage current density. The magnetic behavior of the ceramic samples indicated suppression of antiferromagnetic ordering, observed through the shape of hysteresis curves and the increase in magnetization, which can be attributed to the weakening of geometrical frustration. The observed enhancement of weak ferromagnetism in samples depended on the dopant type and concentration.

#### Application of powder metallurgy in the production of the copper-based material

<u>Marko Simić</u>, Emilija Nidžović, Vladimir Pavkov, Jelena Stašić, Jovana Ružić Department of Materials, "Vinča" Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, PO Box 522, 11001 Belgrade, Serbia

Copper-based materials are integral to various industries due to their remarkable properties, including electrical conductivity, strength and thermal stability. These materials have proven to be indispensable in industries such as marine, aerospace and construction. In this study, a Cu 2 wt.%-Zr 0.6 wt.%-B composite material was designed using powder metallurgy techniques. In order to get a viable material, it was subjected to mechanical alloving (MA), cold pressing. and sintering. Each of these steps highly affect the properties of the final composite material. Different parameters were taken into account for the MA process, including the ball to powder ratio (1:10 and 1:15), milling time (20h, 30h) and the weight ratio of the milling balls (uniform size (6 mm) and different sizes (6 mm, 10 mm, 25 mm)). Optimal results were obtained with a pressure of 350 MPa and for the holding time of 5 min for the cold pressing process. Holding the applied pressure for a particular duration allows the particles to rearrange and adhere to each other. It was established that 5 min was an ideal time for the consolidation of the powder. For the sintering process, a few different temperatures were tested, and the best results were obtained at 1030 °C. The microstructural parameters were analyzed using X-ray diffraction. It was noted that 1:15 MA powders had lower crystallite size values compared to 1:10 MA powders. Strain values were lower for 20h of MA compared to 30 h for 1:10 MA powders, while they were the same for 1:15 MA powder. The ball-to-powder ratio was identified as an important factor in increasing the dislocation density in MA powders, where higher dislocation density values were reached for a 1:15 ratio compared to 1:10, for the same MA duration. The size of milling balls also plays a crucial role in the MA process, as uniform-sized balls provide higher dislocation density values compared to different sized balls. Therefore, the best results for dislocation density were obtained for 1:15 powders after 30h of mechanical alloying with the uniform-sized balls.

*Acknowledgments*: This research was supported by the Science Fund of the Republic of Serbia, Grant No. 7365, Development of dispersion-strengthened metal-based materials for applications in fusion reactor – DisSFusionMat; and by the Ministry of Education, Science and Technological Development of the Republic of Serbia, Contract No. 451-03-66/2024-03/200017.

#### Processing of boron carbide ceramic reinforced with silicon carbide whiskers

Branko Matović, Aleksa Luković

Centre of Excellence-CextremeLab, Vinča Institute of Nuclear Sciences – National Institute the Republic of Serbia Vinča, University of Belgrade, Serbia

Boron carbide ceramics reinforced with silicon carbide fibers ( $B_4C$ -SiCf) were produced via spark plasma sintering, with SiCf content ranging from 2.5 to 10 wt.%. Heat treatment was carried out using the Field Assisted Sintering Technique (FAST) for Spark Plasma Sintering (SPS) at temperatures of 1800 and 2000°C for 5 minutes, under a pressure of 70 MPa in an argon atmosphere. Heating and cooling rates were set at 100 and 50 °C/min, respectively. This study explored the impact of initial powder ratios on sintering behavior, relative density, microstructural development, and mechanical properties of the composites.

Results showed that the sintered ceramics contained only the initial compounds,  $B_4C$  and SiC phases. Scanning Electron Microscopy (SEM) images revealed densely compacted  $B_4C$  and SiC grains in the sintered composites, with a uniform distribution of both phases.

The highest relative density (> 99 %) was achieved in the sample with 95 %  $B_4C$  and 5 % SiCf, sintered at 2000 °C. Microhardness values of the composites ranged from 31 to 43 GPa, depending on constituent content and densification temperature, with the maximum microhardness found in the composite with 95 %  $B_4C$  sintered at 2000 °C.

To assess the composites' performance under extreme conditions, ablation resistance was evaluated using a flowing oxyacetylene torch test. The material containing 5 wt.% SiCf showed superior ablation resistance compared to other compositions. The study concluded that the SPS technique is highly effective for densifying additive-free  $B_4C$ -SiCf ceramic composites, exhibiting promising properties for applications in extreme radiation environments.

# Structure and dielectric behavior of BNT-BT piezoceramics obtained by hydrothermally synthesized powders

Andrea Lazić<sup>1</sup>, Jelena Vukmirović<sup>1</sup>, <u>Iva Toković<sup>1</sup></u>, Marija Milanović<sup>1</sup>, Branimir Bajac<sup>2</sup>, Elvira Toth<sup>3</sup>, Zeljka Cvejić<sup>3</sup>, Vladimir V. Srdić<sup>1</sup> <sup>1</sup>Faculty of Technology Novi Sad, University of Novi Sad, Bulevar Cara Lazara 1, Novi Sad, Serbia

<sup>2</sup>Institute Biosense, University of Novi Sad, Dr Zorana Đinđića 1, Novi Sad, Serbia <sup>3</sup>Faculty of Sciences, University of Novi Sad, Tra Dositeja Obradovića 3, Novi Sad, Serbia

In the modern world, the need for sustainable and efficient energy sources is becoming more and more pronounced. Traditional energy sources, such as fossil fuels, have a negative impact on the environment and have limited reserves, which encourages research into alternative methods for energy production. Piezoelectric materials represent an innovative solution that enables the conversion of mechanical energy from the environment directly into electrical energy. However, there are significant limitations in the use of piezoelectric materials, especially PZT ceramics, due to their toxicity. This creates a strong need to develop alternative lead-free piezoelectric materials.

Bismuth sodium titanate (BNT) systems have been widely investigated over the past decade due to their piezoelectric properties. However, the presence of the non-piezoelectric pyrochlore phase in BNT remains a significant problem in the processing of this material. This work presents different approaches for the production of BNT and BNT-BT nanopowders using the hydrothermal method. The obtained powders were pressed into pellets and sintered under different conditions to produce dense ceramics. Additionally, the effect of sintering conditions and barium addition on the phase composition, density, and dielectric properties of BNT and BNT-BT ceramics was investigated. By optimizing synthesis parameters, thermal treatment, and the amount of barium, the secondary pyrochlore phase was completely eliminated, and pure BNT and BNT-BT phases were obtained.

# The impact of sintering parameters on the physical properties of ceramic samples obtained by andesite basalt powder

<u>Vladimir Pavkov</u><sup>1</sup>, Gordana Bakić<sup>2</sup>, Vesna Maksimović<sup>1</sup>, Aleksandar Maslarević<sup>2</sup>, Bratislav Rajičić<sup>2</sup>, Nenad Milošević<sup>2</sup>, Aleksa Luković<sup>1</sup> <sup>1</sup>Department of Materials Science, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia <sup>2</sup>Faculty of Mechanical Engineering, University of Belgrade, Belgrade, Serbia

Contemporary development of materials prioritizes environmentally friendly and lightweight materials with outstanding physical-mechanical properties fabricated from low-cost natural raw materials that are readily available. In this regard, basalt has emerged as a leading contender. Basalt is a natural igneous rock that can be found in large quantities worldwide, including in Serbia. It is classified as a non-toxic and eco-friendly material, which makes it highly suitable for wide use in construction and industry.

Andesite basalt aggregate from the "Donje Jarinje" site in Serbia was used to produce highdensity ceramic materials. Powder metallurgy was used as a technological process. This technology process involved dry grinding (30 min), manual homogenization (10 min), cold uniaxial pressing (50 MPa), isostatic pressing (230 MPa) of powder, and sintering. Sintering was performed at temperatures 1040, 1050, 1060, 1070 and 1080 °C for 1 hour in the air. This research determined that the highest density of ceramic material from andesite basalt powder is obtained after 1 hour of sintering in the air at 1060 °C. The sample achieved a relative density of 99.5 %. The shrinkage after sintering was 12.8%, while the weight loss was 2.9 % [1]. It is essential to point out that the samples' colour changed after sintering, which was observed by visual control. Due to sintering in the air, hematite formations occurred in the samples, which was confirmed by XRD analysis. With increasing temperature, the colour of the sintered samples changed from light reddish-brown to dark brown. The colour of the sample as a parameter can enable easier monitoring of the production process and indicate the density of the material, i.e. the quality of the manufactured part.

#### **References:**

 Pavkov, V.; Bakić, G.; Maksimović, V.; Cvijović-Alagić, I.; Prekajski Đorđević, M.; Bučevac, D.; Matović, B. High-density ceramics obtained by andesite basalt sintering. *Process. Appl. Ceram.* 2022, 16, 143–152.

#### High-temperature humidity sensing ability of rare-earth-doped barium cerate

<u>Aleksandar Malešević</u>, Aleksandar Radojković, Jelena Mitrović, Milan Žunić, Olivera Zemljak, Sanja Perać, Zorica Branković, Goran Branković University of Belgrade, Institute for Multidisciplinary Research, Center of Excellence for Green Technologies, Kneza Višeslava 1, 11030, Belgrade, Serbia

Acceptor-doped perovskites with large lattice constants have been known as proton conductors. The ability to conduct protons at high temperatures makes them suitable for humidity sensors in a high-temperature environment. In this study, the rare-earth-doped barium cerate powders were synthesized by the auto-combustion method and processed into thick porous films (60 to 70 % porosity) to investigate the water vapor sensing properties in the 400 to 700 °C temperature range. All samples showed a stable sensitivity to water vapor in the whole temperature range, expressed as impedance ratio in dry and wet argon ( $|Z|_{dryAr} / |Z|_{wetAr}$ ), and were able to detect 0.03 vol.% of water vapor at 550 °C within the impedance range of 10 k $\Omega$  at 100 Hz. The sensitivity values increased with the partial pressure of water and decreased with the temperature, whereas the maximal value of 3.41 reached the BCEu10 sample at 550 °C and  $p_{H_2O} = 4.28$  kPa.

### Sintering behavior of Mo-based metal-matrix composite

<u>levgen Solodkyi</u><sup>1,2</sup>, Manja Krüger<sup>1</sup>
 <sup>1</sup>Otto von Guericke University Magdeburg, Universitätsplatz 2, Magdeburg 39106, Germany
 <sup>2</sup>Igor Sikorsky Kyiv Polytechnic Institute, 35 Politechnichna Str., Kyiv, 03056, Ukraine

Metal-matrix composites (MMCs) are advanced materials and widely used in various fields of industry, where high physical, mechanical and functional properties are of vital importance. Mo-based alloys show great potential for ultrahigh-temperature applications because of their high melting points, high stiffness, and low coefficient of thermal expansion. However, the insufficient strength at elevated temperatures, low-temperature brittleness and poor oxidation resistance are the main concerns for Mo-rich alloys in practical use. Toward this end, fabricating Mo-based MMCs reinforced with multi-phase Mo-Si-B material and  $Ti_5Si_3$  ceramic particles have been aimed to solve the above-mentioned problems. Moreover, the use of powder metallurgy technology makes it possible to obtain a uniform distribution of reinforcing particles in the molybdenum matrix.

The activated pressureless sintering (PLS) of MMCs (Mo- matrix reinforced with multi-phase Mo-9Si-8B particles as well as  $Ti_5Si_3$  ceramic particles) by the addition of Ni was applied. The influence of technological parameters of PLS and SPS (temperature and holding time) and the concentration of the reinforcing particles were investigated. Based on the analysis of the microstructure and phase composition the main mechanisms of sintering and formation of the composite microstructure were established. The mechanical properties of dense composite materials were also studied.

In order to improve sinterability of Mo-matrix composite core-shell  $Ti_5Si_3$ -Mo powders were successfully synthesized by reducing of ammonium molybdate (para) tetrahydrate with hydrogen and glycerol, respectively. As a result, the  $Ti_5Si_3$  core was coated with submicron and nanosized Mo particles. It was shown that powders with a core-shell structure are densified up to a temperature of 1330 °C, while the mechanical mixture of commercial powders at this temperature only begins to densify. Fractographic studies have shown the presence of a pseudo-brittle fracture mechanism for the metal matrix composite (MMC), which was sintered by SPS of the core-shell  $Ti_5Si_3$ -Mo powder synthesized by reduction with glycerol.

## AUTHOR INDEX

## Α

Adomaviciūtė-Grabusove S	146
Anđelković Lj	61, 64
Andrushchak A	106
Antić A	66
Antonov V	105
Aoki M	145, 149

## В

Babić B	
Baginskiy I	27, 40, 54, 96, 120
Bajac B	
Bajat J	122
Bajić D	
Bajuk-Bogdanović D	
Bakić G	
Balać I	
Balanč B	
Banićević I	
Barać N	117
Barceló E	117
Barvinchenko V	
Basak A	
Bassett L	
Bazarnik P	
Bekenov L	105
Beladi Mousavi M	
Belec B	59
Belošević-Čavor J	115
Beneš P	
Berger F	73
Bernard-Granger G	
Bezkrovnyi O	
Bhatia P	
Blawert C	46, 71
Boczkal G	
Bojić L	
Borodušķis M	
Bozbey Y	
Božić D	
Branković G	155, 157, 162
Branković Z	155, 157, 162
Brus J	124, 125
Büber E	
Buchczik D	73
Buryy O	106

## С

Caro P	120
Cengeri P	144
Chacko L	23
Chen B	32
Chen L	151
Cheng H-M	11
Chorna I	40, 120
Chudinovych O	81
Chyzhyk G	
Cortes E	45
Cui Y	4
Cui Yi	4
Cvejić Z	160
Cvijović-Alagić I	94
Czaja P	
Czernek, J	125

## Č

Čaplovičová M	96
Černeková N	93

## Ć

Ćirić-Marjanović	G	85,	107
------------------	---	-----	-----

## D

Daković A	
Damjanović-Vasilić Lj	
Dascau H	
De Bona E	
Deineka V	
dePedro-Embid I	21
Diedkova K	
Dimić-Mišić K	
Dimitrijević I	51
Dinić A	
Dinić I	
Djerdj I	80
Dmytrivna Pinchuk N	
Dominko R	
Doreau F	147
Drdlíková K	
Drndić M	10
Drozdenko D	
Duguay C	147
Dukhnovskiy S	40, 54, 96, 120
Dybkova S	

## Ð

Đokić V	122
Đorđević V	
Đuknić M	
Đurđić Mijin S	21

## Ε

Elhmali HT	
Enia E	
Erčić J	86
Eremenko ZE	

## F

Feia O	
Fenech M	145, 149
Feng X	
Finšgar M	80
Fortes Palley B	112
Fraser HL	139

## G

Gabrič M      31        Gajica G      66        Galaţanu S-V      103        Galstian I      .74, 76, 94
Gandara M
Gavrilov N
Gazder AA
Ge K
Gezović Miljanić A 37, 102
Gnilitskyi L
Gogotsi O 27, 39, 40, 54, 68, 69, 96, 120, 146
Gogotsi Y5, 45, 54, 55, 146
Goncharuk O 116
Grbović Novaković J 59
Gregorczyk M 48
Grilc M 31, 67
Grine L
Gröbmeyer F 45
Gruber C 45
Grudić V56, 57, 102
Grujić A 89
Grujičić M62, 63, 82
Guillen Pineda RM 156
Guillon O 133
Gusdorff J 10
Guzenko N 116
Gyergyek S 79

## Н

Harth F	67
Herber M	22
Hersam MC	13
Hill EH	22
Hersam MC	13

Hočevar B	31
Hodan J	109
Holubnycha V	127
Horky J	144
Hryhorova T	113
Hu Y-J	55
Huang Y	41
Huo S	
Huš M	31
Husak Y	68, 96

## I

Ilić DI	84
Imani M	
Inman A	45
Ippolito S	54
Isailović JN	66
Ivanovska A	47
Ivanovski V	115

## J

Jaćimović Ž	
Jakovljević T	
Janaćković Đ	
Jančić Heinemann R	
Jančić I	
Janković M	
Janković R	
Janošević Ležaić A	
Jardim P	
Jasik K	
Jatsyk B	
Jeftić B	
Jekabsons K	
Jelić M	
Ješić D	
Jovančićević B	
Jovanović M	
Jovanović S	
Jovanović Z	
Jovović N	
Jurak M	
Julak ///	

## Κ

Kadlecová Z	93
Kang S-JL	132
Kania H	100
Kania K	73
Kapidžić A	115
Kapidžić M	
Kardaszuk E	
Kastratović S	57
Kaurkovska V	54
Kausaite-Minkstimiene A	111
Kazakova O	
Keneipp R	10

I/ AA	
Kerber M	
Kernosenko L	
Kijevčanin M	
Klishchova Z	40, 120
Kluczyński J	
Klym H	
Kobera L	124
Kochetov G	101
Kojčinović A	67
Kojčinović J	80
Kojić S	
Kolesnichenko V	
Komedera K	105
Konefał M	109
Kónya Z	80
Korica M	
Korniienko O	
Korniienko Va	
Korniienko Vi	39. 68. 69. 96
Kornyushin Y	
Kosmulski M	
Kosović Perutović M	
Koster G	
Kostić M	
Kostiv Y	
Kosturek R	
Koteski V	
Kovač J	
Kovačević S	
	53
Kovalčík A	53 93
Kovalčík A Kovalenko V	
Kovalčík A Kovalenko V Krawczynska A	
Kovalčík A Kovalenko V Krawczynska A Krüger M	53 93 94 24 
Kovalčík A Kovalenko V Krawczynska A Krüger M Krunić T	53 93 94 24 163 90
Kovalčík A Kovalenko V Krawczynska A Krüger M Krunić T Kubova K	53 93 94 24 163 90 124
Kovalčík A Kovalenko V Krawczynska A Krüger M Krunić T Kubova K Kuchař J	
Kovalčík A Kovalenko V Krawczynska A Krüger M Krunić T Kubova K Kuchař J Kudláček J	53 93 94 24 163 90 124 73 73
Kovalčík A Kovalenko V Krawczynska A Krüger M Krunić T Kubova K Kuchař J Kudláček J Kukovecz Á	
Kovalčík A Kovalenko V Krawczynska A Krüger M Krunić T Kubova K Kuchař J Kudláček J Kukovecz Á Kuprin O	53 93 94 24 163 90 124 73 73 73 80 108
Kovalčík A Kovalenko V Krawczynska A Krüger M Krunić T Kubova K Kuchař J Kudláček J Kukovecz Á Kuprin O. Kuraica M	53 93 94 24 163 90 124 73 73 80 80 108 30, 47
Kovalčík A Kovalenko V Krawczynska A Krüger M. Krunić T. Kubova K. Kuchař J. Kudláček J Kukovecz Á. Kuprin O. Kuraica M. Kurko S	53 93 94 24 163 90 124 73 73 80 80 108 30, 47 59
Kovalčík A Kovalenko V Krawczynska A Krüger M Kuchař J Kudláček J Kudláček J Kukovecz Á Kuprin O Kuraica M Kurko S Kushnir O Kuzmenko M	
Kovalčík A Kovalenko V Krawczynska A Krüger M. Krunić T. Kubova K. Kuchař J. Kudláček J Kukovecz Á. Kuprin O. Kuraica M. Kurko S	

## L

Lalatović K	
Langdon TG	41
Łasica W	48
Lastivka O	101
Lavrič Ž	
Lazić A	
Lazić S	
Lazić V	90
Lebed V	74
Leka Z	
Len E	

Len Y	74
Leniec G	
Lewandowska M	24, 41
Li J-F	135
Likozar B	31, 58, 67
Lipkovska N	126
Lisova O	74
Lisyte V	111
Lobunets T	
Lojpur V	60
Lukić J	
Luković A	159, 161
Luković Golić D	

## Lj

Ljujić B	 97
LJUJIC B	 

## Μ

Маса К	148
Madej J	94
Maksimović V	
Małek M	48
Malešević A	155, 157, 162
Mančić L	
Manzanares-Palenzuela CL	43
Marek A	100
Mares Barbosa S	109
Marinković BA	83
Marković M	
Marguis F	
Maślana K	20
Maslarević A	
Matić T	
Matija L	52
Matović B	
Matthews K	45
Mazo I	
Međo BI	72
Melero H	156
Mentus S	
Messer O	44
Metin Ö	110
Miądlicki P	35
Miĥajlović D	122
Mijailović D	104
Mijowska E	20, 36
Milanović M	160
Milić JV	19
Milikić J	
Milivojević M	
Milošević Ma	47
Milošević Mi	26
Milošević MS	72
Milošević N	
Minor AM	
Miranda-Castro J	8

Mišurović J	
Mitrović J	
Mizeracki J	
Mladenović D	
Mojsilović K	46, 71, 77
Mojsilović S	
Monastyrov M	
Mondal B	
Mraković A	61, 64
Mravik Ž	
Murakami D	

## Ν

Nakano N	145, 149
Naseri R	150
Nedović V	70
Niaura G	
Nicolosi V	
Nidžović E	
Niessen F	150
Nikitović Ž	75
Nikolić G	52
Noga H	105
Novohatskyi M	
Nykyruy Y	105

## 0

Obradović B	25, 26, 29
Obradović Br	
Obradović M	
Obradović N	
Obuch J	125
Ogórek R	
Olevsky E	
Olifan O	81
Oliveira A	120
Osmokrović A	
Ostash O	
Ožegović M	65

## Ρ

Pajić D	
Palusińska-Szysz M	
Panić V	
Pantić T	
Papić M	
Pašti I	85, 86, 107
Pastuszak K	
Paunić M	103
Pavelkova M	
Pavkov V	
Pavlišič A	
Pavlova E	
Pavlović V	61, 64
Pejčić M	
Perać S	

Pereloma E150
Perišić S
Perju A
Petković D
Petrichenko O27
Petrović B96
Petrović J
Petrović M95, 119
Petrović R
Piecuch A91
Pietrusewicz K20
Pinchuk N123
Piotrkiewicz P
Počuča-Nešić M155
Podhurska V108
Podlogar M155, 157
Pogorevc R
Pogorielov M 27, 38, 39, 40, 68, 69, 96, 120
Pogrebnjak AD96
Pokorný P100
Poltoratska T12
Popov A111, 146
Potashna M54
Pratsinis SE
Prikhna T94
Prvulović M
Prysiazhna O94
Pshenychnyi R122

## Q

Quang Lê	è H	30
----------	-----	----

## R

Rac V	
Radinović K	
Radisavljević A	
Radmilović V	
Radojević V	89, 95, 104, 119
Radojković A	
Radonjić B	
Radosavljević ZM	72
Radovanović Ž	25
Radović M	
Ragulya AV	
Rajičić B	
Rakočević L	112
Raković D	
Ramanaviciene A	111, 146
Ramanavicius A	
Ramanavicius S	146
Ranković M	
Raspopović Z	75
Ratzker B	
Rems E	
Riedel R	
Riekstina U	

Ristić M	
Rmuš Mravik J	59, 82
Rogach AL	
Rondović K	
Roshchupkin A	
Roslyk I	40, 54, 96, 120
Rotter M	
Rud M	
Ružić J	

## S

Sablinskas V	146
Sahraoui B	106
Sajti L	144
Salamon D	143
Samchenko D	101
Samchenko Y	. 116. 123
Sapauskiene M	
Sápi A	
Sarmento Gonçalves E	112
Savić M	
Savvakin D	
Schafler E	
Schröder T	
Schwarzbauer J	66
Sedmak AS	
Sedminek A	
Serdechnova M	46 71
Setman D	
Sglavo VM	136
Shcherba I	
Shevchenko M	
Shevchuk K	
Shmatkov A	
Shulga D	
Shumilin S	
Shyrokov O	
Sielicki K	
Simić M	
Simka W	
Simon P	
Simović B	
Sinclair R	
Skalar T	
Smiljanić D	
Śnieżek L	
Sobierajska P	91
Sokol M	
Solodkyi I	
Spreitzer M	
Spurling D	
Srdić VV	160
Środa B	
Stajčić A	
Stajčić I	
Staiić-Trošić J	89
Stamenković T	60

Stanisavljević N	70
Stanković D	
Stanković I	52
Starushenko K	
Stašić J	
Steinerová V	100
Stelmakh S	123
Stijepović M	117
Stojadinović S	46, 71, 77
Stojanović DB	
Stojanović S	46, 77, 88
Stojković Simatović I	63
Stojkovska J	26, 29, 92
Stolarczyk A	
Stolić P	82
Strachota A	109
Strachota B	109
Suchecki P	24
Sulkowski B	144
Svircev Z	47
Swanson D	15
Sych O	123
Synytsia A	123
Szalai A	43
Szenti I	80
Szewczuk-Karpisz K	116
Szyszka K	91

## Š

Šarić S	80
Šenjug P	
Šetraičić JP	84
Šliukić B	88 110 112
Šuljagić M	

## Т

Taberna P-L	
Tadić M	61, 64
Tadić N	77
Tadić V	119
Talaikis M	146
Targońska S	91
Tatar D	80
Ther O	156
Tian M	80
Timotijević M	51
Tinnefeld P	43
Todorović M	65
Toković I	160
Tomila T	
Toprek, D	115
Torchilin V	3
Torrente K	
Toth E	
Trajković ID	72
Trstenjak U	

## U

Ugrinović V	
Ullah H	80
Umićević A	115
Urbanova M	124, 125
Uskoković D	105
Uskoković P	92, 95, 104

## V

Valášek D	
Varava Y	
Varvarin M	74
Vasilić R	
Vavřík D	
Veljović Đ	
Vesel A	
Vižintin A	
Vojisavljević K	
Vojtová L	
Volić M	
Vorotytskyi P	123
Vronska Y	123
Vujković M	37, 56, 57, 102
Vukićević EN	
Vukmirović J	160
Vuković M	
Vuksanović M	

## W

Wachowski M	
Waloszczyk N	68, 96
Wang J	45
Wang Y	
Warren K	39
Wiglusz RJ	

Wirawan R	145, 149
Wróblewska A	35
Wu Y	137

## Y

Yadav M	80
Yalyzhko M	
Yamashita K	
Yanko I	
Yanovska A	
Yurchenko Y	

## Ζ

Zabrodin P113, 121
Zahorodna V 27, 39, 40, 54, 68, 69, 96, 120
Zając G73
Zamula M
Zayats AV
Zdeněk S
Zehetbauer MJ144
Zemljak O155, 157, 162
Zhak O105
Zheludkevich ML46, 71
Zhou Y151
Zielinkiewicz K36
Zielińska B35
Zlatičanin B
Zschech E9
Zukauskas S146
Zygmuntowicz J34

## Ž

Žemlička J	121
Žunić M.	162
Żurowski R	34

# TWENTY-FIFTH JUBILEE ANNUAL CONFERENCE ON MATERIAL SCIENCE YUCOMAT 2024

&

# THIRTEENTH WORLD ROUND TABLE CONFERENCE ON SINTERING XIII WRTCS 2024

Hunguest Hotel Sun Resort, Herceg Novi, Montenegro September 2 to 6, 2024

# APPENDIX

## to the

# Program and Book of Abstracts

Organised by Materials Research Society of Serbia & International Institute for the Science of Sintering

Endorsed by Federation of European Material Societies

# YUCOMAT Oral Presentations

### O.S.II.B.7

## Non-destructive testing of composite helmets using ultrasonic thermography

Waldemar Swiderski Military Institute of Armament Technology, Zielonka, Poland

Personal ballistic covers, i.e. composite helmets (and armor vests), use multi-layer composite materials, which are woven materials (including aramid fibers) connected with plastic as a binder. These types of materials are characterized by the fact that they are light, resistant to corrosion, and can be easily formed, which allows them to be adapted to the surface they are intended to protect. Light ballistic shields are most often several to a dozen or so millimeters thick. Defects that may occur in multi-layer composite materials include defects resulting from the technological process and use. These defects affect the properties of the composites, i.e. their number, dimensions, shape and arrangement. Technological defects are related to the method of producing the cover and arise during an incorrectly conducted technological operation. Defects that may occur in this type of composite materials include: inaccuracies in gluing the composite layers, disbonding, thin gas gaps, most often filled with air, delam inations occurring between the composite layers, occurring during impacts caused by impacts, fragments and shell fire as a result of destructive ballistics tests, material discontinuities, inclusions of foreign materials, flat cracks, etc. The above-mentioned defects may also occur together. Each composite helmet is individual equipment and is used differently by each user. In addition to objective factors affecting its efficiency, such as climatic conditions, its technical condition after many years of operation is also influenced by the user himself. Due to the complicated shape of composite helmets, many non-destructive testing methods are not effective in detecting defects that may occur in them. Among the tests carried out at the Institute using various non-destructive testing methods for helmets, the best results were obtained using ultrasonic thermography. Ultrasonic infrared thermography uses an ultrasonic signal as an excitation source, which leads to thermal excitation of samples and significantly higher temperatures in defective areas compared to adjacent areas without defects. The ultrasonic infrared thermography method has many important advantages over ordinary thermography. The article presents the results of experimental testing.

Presentation time Friday, September 6, 2024, 11<sup>00</sup> - 11<sup>15</sup> Second YUCOMAT Oral Session, Main Conference Hall

# YUCOMAT Poster Presentations

#### P.S.I.A.5

## Diversifying Properties of Ti<sub>3</sub>AlC<sub>2</sub> MAX Phase: Doping with Nb and Mo by Molten Salt-Shielded Synthesis

Filipa M. Oliveira<sup>1</sup>, Nima Amousa<sup>2</sup>, Amutha Subramani<sup>1</sup>, Jan Luxa<sup>1</sup>,

Chenrayan Senthil<sup>3</sup>, Zdeněk Sofer<sup>1</sup>, Jesus Gonzalez-Julian<sup>2</sup> <sup>1</sup>Department of Inorganic Chemistry, Faculty of Chemical Technology, University of Chemistry and Technology Prague, Technická 5, 166 28 Prague 6, Czech Republic, <sup>2</sup>Chair of Ceramics, Institute of Mineral Engineering (GHI), RWTH Aachen University, Forckenbeckstrasse 33, 52074 Aachen, Germany, <sup>3</sup>Department of Energy Engineering, Gyeonsang National University, Jinju-si, Gyeongnam, 52725, South Korea

This study employs the molten salt-shielded method to dope the  $Ti_3AlC_2$  MAX phase with Nb and Mo, aiming to expand the intrinsic potential of the material. X-ray diffraction confirms the preservation of the hexagonal lattice structure of  $Ti_3AlC_2$ , while Raman and X-ray photoelectron spectroscopic analyses reveal the successful incorporation of dopants, with subtle yet significant alterations in the vibrational modes and chemical environment. Scanning electron microscopy with energy-dispersive X-ray spectroscopy characterizations illustrate the characteristic layered morphology and uniform dopant distribution. Density functional theory simulations provide insights into the modified electronic structure, displaying changes in carrier transport mechanisms and potential increases in metallic conductivity, particularly when doping occurs at both the M and A sites. The computational findings are corroborated by the experimental results, suggesting the enhanced material may possess improved properties for electronic applications. This comprehensive approach not only expands the MAX phase family but also tailors their functionality, which could allow the production of hybrid materials with novel functionalities not present in pristine form.

Presentation time **Tuesday, September 3, 2024 First YUCOMAT & WRTSC Poster Session, National Restaurant Jadranka Terrace** Competition for the best Poster Presentation of young researchers Session: 08<sup>00</sup> - 09<sup>45</sup> YUCOMAT SYMPOSIUM A: ADVANCED METHODS IN SYNTHESIS AND PROCESSING OF MATERIALS

#### P.S.III.C.22

## Protective coating for current collector materials of direct liquid fuelled molten carbonate fuel cell

Mariia Shved<sup>1</sup>, Viktoriya Podhurska<sup>1</sup>, Oleksandr Kuprin<sup>2</sup>, Jaroslaw Milewski<sup>3</sup>

<sup>1</sup> Karpenko Physico-Mechanical Institute of the NAS of Ukraine, Lviv, Ukraine <sup>2</sup> National Science Center "Kharkiv Institute of Physics and Technology" of NASU, Kharkiv, Ukraine <sup>3</sup> Warsaw University of Technology, Warsaw, Poland

Due to the growing problem of global warming, molten carbonate fuel cells (MCFCs) are considered a promising technology for producing clean energy from hydrogen and various fuels such as natural gas, biogas and syngas. MCFCs have a high efficiency of up to 60% and do not produce pollutants, which makes them an attractive alternative to conventional energy generation methods. The MCFCs powered directly by liquid hydrocarbon fuels is an alternative to power generators based on internal combustion engines or gas turbines, desirable for applications away from fixed electricity sources and the fuel grid, as well as for other portable applications.

One of the main challenges is the degradation of MCFC components. The review of the literature shows that one of the main sources of MCFC degradation, which affects the performance and durability of fuel cells, is the corrosion of MCFC parts, mainly current collectors and interconnectors/bipolar plates. Interconnects/bipolar plates provide the supply of the operating gas environment and current transportation in fuel cell stacks. As materials for interconnects, highly alloyed steels, with oxidation resistant and electrically conductive coatings based on spinel or perovskite are traditionally used. One of the methods of protecting and improving the corrosion properties of steels is the application of coatings based on nitrides. The aim of the work is to study the service properties of thin (0.5 mm) stainless steel interconnects with nanostructured coatings of the Cr-N, Cr-Ti-N and Ti-Al-Gd-N systems at 600C in the air.

The coatings were deposited on polished 304L stainless steel specimens using a Cr, Ti-Al, Ti-Al-Gd cathode and the vacuum arc method. Oxidation resistance and electrical conductivity of coatings after long-term (1000 h) holding at 600°C in air were studied. Electrical conductivity of obtained coating was  $1.7...3.5 \cdot 10^5$  S/m.

The work was supported by the NATO project SPS G6292 "Direct liquid fuelled Molten Carbonate Fuel Cell for Energy Security (DIFFERENT)".

Presentation time **Thursday, September 5, 2024 Third YUCOMAT Poster Session, National Restaurant Jadranka Terrace** Session: 08<sup>00</sup> - 09<sup>45</sup> YUCOMAT SYMPOSIUM C: NANOSTRUCTURED MATERIALS

# WRTCS Oral Presentations

## Entropy as an Order Parameter in Thermodynamics

Yuri Kornyushin

Maître Jean Brunschvig Research Unit, Chalet Shalva, Randogne, CH-3975

Rudolf Clausius had introduced Entropy as a measure of order/disorder (that is as an Order Parameter) in the early 1850<sup>th</sup>.

In 1937 Lev Landau had introduced another order parameter also. The order parameter of Landau is different in every specific case. It should be determined for every specific case independently. Entropy is a universal parameter, all the same for every specific case. This is a great advantage.

The author started to use Entropy as an order parameter in the early 1980<sup>th</sup>. This technique allowed the author to formulate a general formulation of Thermodynamics of Metastable States [1].

The general theory was reported as a key lecture on the 13<sup>th</sup> Colloquium on Thermophysical Properties in Boulder, Colorado, USA, and it is available free for everybody on The Net Advance of Physics site of MIT in Metastability topic.

Reference:

1. Kornyushin, Y. Phenomenological Thermodynamics of Metastable States. J. Non Equilib. *Thermodyn.* **2000**, *25*, 15–30.

Presentation time Wednesday, September 4, 2024, 17<sup>15</sup>- 17<sup>30</sup> Second WRTCS Oral Session, Main Conference Hall

# ACKNOWLEDGEMENTS



FEDERATION OF EUROPEAN MATERIALS SOCIETIES















# WELCOME TO Twenty-sixth Annual Conference YUCOMAT 2025

Herceg Novi, Montenegro, September 1 to 5, 2025.





