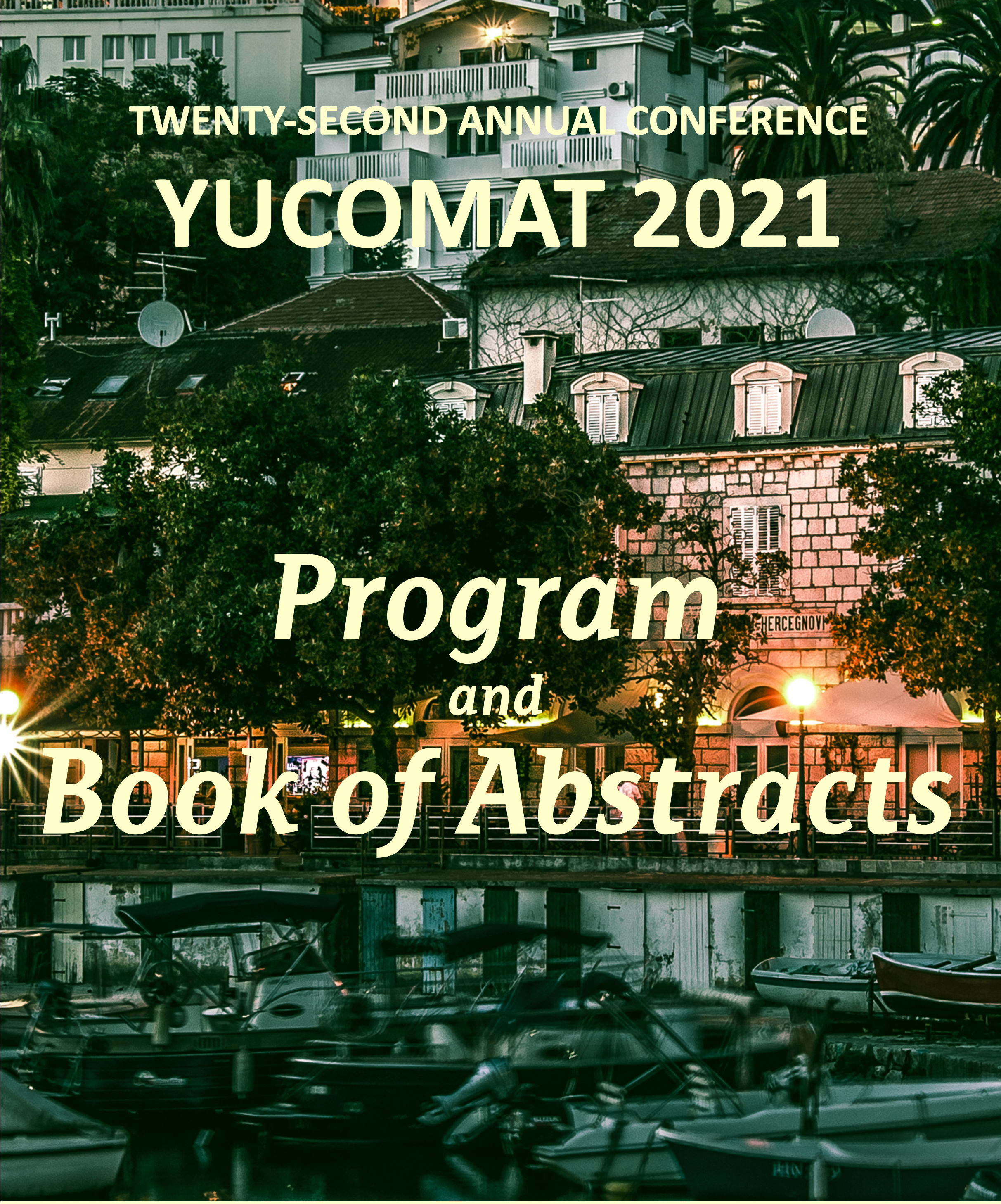

TWENTY-SECOND ANNUAL CONFERENCE

YUCOMAT 2021

Program
and
Book of Abstracts

endorsed by

FEMS
FEDERATION OF EUROPEAN
MATERIALS SOCIETIES

SERBIA MRS
Materials Research
Society of Serbia

TWENTY-SECOND ANNUAL CONFERENCE

YUCOMAT 2021

Hunguest Hotel Sun Resort, Herceg Novi, Montenegro
August 30 - September 3, 2021
http://www.mrs-serbia.org.rs

Program
and
Book of Abstracts

Organised by:
Materials Research Society of Serbia

Endorsed by:
Federation of European Material Societies

CIP - Каталогизацијаупубликацији
НароднабиблиотекаСрбије, Београд

66.017/.018(048)

DRUŠTVO za istraživanje materijala Srbije (Beograd). Godišnja konferencija (22 ; 2021 ; Herceg Novi)
Programme ; and the Book of abstracts / Twenty-second Annual Conference YUCOMAT 2021 Herceg Novi, Montenegro, August 30 - September 3, 2021 ; organised by Materials Research Society of Serbia ; [editor Dragan P. Uskoković]. - Belgrade : Materials Research Society of Serbia, 2021 (Herceg Novi : Biro Konto). - XXXIII, 146 str. : ilustr. ; 23 cm

Tiraž 150. - Bibliografija uz pojedine apstrakte. - Registar.

ISBN 978-86-919111-6-4

а) Наука оматеријалима-- Апстрактиб) Техничкиматеријали—Апстракти

COBISS.SR-ID 44447497

Title: THE TWENTY-SECOND ANNUAL CONFERENCE
YUCOMAT 2021
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; hhttp://www.mrs-serbia.org.rs

Editor: Prof. Dr. Dragan P. Uskoković

Technical editor: Jasmina R. Jevtić

Typesetting
and prepress: Dr. Aleksandar Dekanski
Cover page: Nenad Ignjatović
Covers: Images on front & back covers are the property of MRS Serbia

ISBN 978-86-919111-6-4

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: 150 copies. The end of printing: August 2021

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ABSTRACTS

WELCOME SPEECH BY THE PRESIDENT OF MRS-SERBIA

Dear Attendees,

It is my great pleasure to greet you on behalf of the Conference hosts and wish you a solid program, lots of happiness and good health, which we all need in these times. Not a single prior YUCOMAT Conference has been organized with as much uncertainties as this one. Some remember the Third YUCOMAT Conference held right after the NATO bombing of Serbia and Montenegro, which lasted from the end of March 1999 until mid-June that same year. That Conference was held with a single foreign participant – Giovanni Battiston, CNRS, Padua, Italy, who said back then, “I promised that I would come and now I am here”. Last year was the first one to have a YUCOMAT Conference cancelled, not long before it was scheduled to be held, after it was clear that the risk for the participants would be too large.

As we reached the 100th submission during June and July this year, we decided that the Conference should be organized, hoping that the positive epidemiological situation would continue throughout the summer and that all of us would do it all to respect the measures in place. A number of plenary lecturers had to cancel their lectures and postpone them for the next year (YUCOMAT, August 29 – September 2, 2022), considering the travel limitations in many countries. There are still around 10 plenary lecturers in the Program, some of whom would talk here and some of whom sent their presentations, which are posted on the MRS webpage. Out of 100 authors who will present their research orally and via posters, the majority are from Serbia, around 30 %, followed by participants from Poland, Czech Republic, Slovenia and Russia, accounting for about 40 % in total, whereas no other country has more than 3-4 participants. The coronavirus has done its fair share and as a result we have a very different structure compared to earlier years, when the predominant participants were from USA, Korea, Taiwan and the Far East.

After five winners of the Big Award of our Society for the lasting and outstanding contribution to materials science who originated from the region of former Yugoslavia, the last year’s winner was Robert Sinclair, Charles M. Piggot Professor in the School of Engineering at Stanford and the first the win this award after its internationalization and opening to all our members. Robert Sinclair gave a significant contribution to our field and our Society as a long-term President of the International Advisory Board and a participant at all recent YUCOMAT Conferences. Since the last year’s Conference was not held and was postponed and since Bob could not attend this year’s conference, he sent his talk and the certificate and the medal will be given to him next year. This year’s winner of the Award is Prof. Yuri Gogotsi, director of the Drexel Nanotechnology Institute, for his contribution to the field of nonoxide materials with a special emphasis on MAXene family of 2D metal carbides and carbonitrides and a long-term successful cooperation with our country through MRS-Serbia and the International Institute for the Science of Sintering. The decision for both winners is found in the Program and the Book of Abstracts.

One of the very important activities of our Society since its beginning was the recognition of the young researchers as Conference participants. As of this year, MRS – Singapore as one of the most active MRS in the world and the one which will be the headquarters of the International Union of MRS (IUMRS) has joined us in the financial segment of this award. Tuesday will be dedicated to this activity and 20 young people will compete for the best oral presentation, whereas in the afternoon 20 of them will compete for the best poster presentation. In both cases we will select 5 best presenters and their names will be announced on Friday at the Conference Closing, whereas the certificates and the financial rewards will be handed to them at the opening of the first following Conference.

This is Tenth YUCOMAT Conference to be held in this Hunguest Sun Resort Hotel. At this very same location, which used to be the Nuclear Center belonging to the Nuclear Commission of former Yugoslavia, starting from 1969, the World Round Table Conferences of Sintering were held, where, just like today, world-renowned scientists from both West and East used to congregate. In the Iron Curtain era, in fact, it was the only place where they could meet. This part of Herceg-Novi is called Topla and some of the most intellectual people from this region have occasioned it. Our famous poet and statesman, Petar II Petrović Njegoš, for example, was educated in a little house near the Church of Saint George, not far from here, whereas directly on the opposite side our Nobel Laureate in literature, Ivo Andric, used to live and work. Our hosts at the Hunguest Hotel maintain the memory of those people and those times by helping us organize these conferences. There is a lot of examples of their highly positive attitude toward this meeting, including the traditional cocktail party they organize on Monday evening, which is always memorable. I hope that this Conference will also go well and will be worth remembering and that we will all happily and healthily return to our homes from it.

Sincerely Yours,
Dragan Uskoković

2020 MRS-SERBIA AWARD FOR A LASTING AND OUTSTANDING CONTRIBUTION TO MATERIALS SCIENCE AND ENGINEERING

We are pleased to announce that the laureate of the **2020 MRS-Serbia Award for a Lasting and Outstanding Contribution to Materials Science and Engineering** is

Prof. Robert Sinclair of the Stanford University, California, USA.

He is awarded for his contribution to electron microscopy applied to materials science and engineering.

This is the decision of the MRS-Serbia Executive Board:
The Executive Board of the MRS-Serbia Presidency, at their meeting on March 30th, 2020, considered the submitted nomination for the MRS-Serbia's 2020 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 January 1, 2020, 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. Ivan Božović (2015 Laureate), Prof. Dr. Gordana Vunjak-Novaković (2016 Laureate), Prof. Dr. László Forró (2018 Laureate) and Prod. Dr. Danilo Suvorov (2019 Laureate), the Executive Board of the MRS-Serbia Presidency took the decision that Prof. Robert Sinclair should be granted MRS-Serbia's 2020 Award for a Lasting and Outstanding Contribution to Materials Science and Engineering.
Prof. Sinclair was nominated by Prof. Dr. Velimir Radmilović, strongly supported by Dr. Slobodan Milonjić, Prof. Dr. Đorđe Janaćković, Prof. Dr Petar Uskoković, Prof. Dr. Nenad Ignjatović, Dr.Smilja Marković, Prof. Dr. Dejan Raković.
Prof. Robert Sinclair's invited plenary lecture "In situ High Resolution Electron Microscopy of Material Reactions, at the Atomic Level" will be presented during the Opening Ceremony of the 22nd MRS-Serbia Annual Conference YUCOMAT 2021, as a Virtual Lecture, starting at 9.00 a.m. on Monday, August 30, 2021.

President of MRS-Serbia, Prof. Dr. Dragan Uskoković
Vice-President of MRS-Serbia, Dr. Slobodan Milonjić
Vice-President of MRS-Serbia, Prof. Dr. Velimir Radmilović
Vice-President of MRS-Serbia, Prof. Dr. Dejan Raković

2021 MRS-SERBIA AWARD FOR A LASTING AND OUTSTANDING CONTRIBUTION TO MATERIALS SCIENCE AND ENGINEERING

We are pleased to announce that the laureate of the **2021 MRS-Serbia Award for a Lasting and Outstanding Contribution to Materials Science and Engineering is**

Prof. Yury Gogotsi of the Drexel University, Philadelphia, USA.

He is awarded for his contributions to the field of non-oxide nanomaterials and specially MXene family of compounds.

This is the decision of the MRS-Serbia Executive Board:
The Executive Board of the MRS-Serbia Presidency, at their meeting on March 13th, 2021, considered the submitted nomination for the MRS-Serbia's 2021 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 January 1st, 2021, and that in the stipulated period of 45 days only one nomination was submitted.

Having received the opinion from the Expert Committee members: Prof. Dragan Uskokovic (President of MRS-Serbia), Prof. Robert Sinclair (Chair of YUCOMAT Conferences International Advisory Board and as 2020 Laureate), Prof. Dejan Rakovic (Vice-President of MRS-Serbia), Dr. Slobodan Milonjić (President of the Council and Member of the Presidency of MRS-Serbia), Prof. Dr. Nenad Ignjatovic (Member of the Presidency and Secretary General of MRS-Serbia) and Prof. Dr. Ivan Bozovic, as 2015 Laureate, Prof. Dr. Gordana Vunjak-Novaković, 2016 Laureate, Prof. Dr.Velimir Radmilović, 2017 Laureate, Prof. Dr. László Forró, 2018 Laureate and Prof. Danilo Suvorov 2019 Laureate, the Executive Board of the MRS-Serbia Presidency took the decision that Prof. Yury Gogotsi should be granted MRS-Serbia's 2021 Award for a Lasting and Outstanding Contribution to Materials Science and Engineering.
Prof. Gogotsi was strongly supported by Prof. Dragan Uskoković, Dr. Slobodan Milonjić, Prof. Yuri Solonin, Prof. Masahiro Yoshimura, Prof. Paul Weiss, Prof. Michael W. Barsoum, Prof. Eugene A. Olevsky and Dr. Vuk Uskokovic.
Prof. Yury Gogotsi's invited plenary lecture will be presented during the Opening Ceremony of the 22nd MRS-Serbia Annual Conference YUCOMAT 2021, starting at 9.00 a.m. on Monday, August 30, 2021.

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
Vice-President of MRS-Serbia, Dr. Smilja Marković
General Secretary of MRS-Serbia, Prof. Dr. Nenad Ignjatović

MRS-Serbia

President of the Council: Slobodan Milonjić
President: Dragan Uskoković
Vice-presidents: Velimir Radmilović, Dejan Raković, Smilja Marković
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International Advisory Board
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YUCOMAT GENERAL INFORMATION

Conference Organising Committee

Chairpersons: Đorđe Veljović, Zoran Jovanović
Members: Branko Matović, Irena Nikolić, Bojana Obradović, Vuk Radmilović, Nebojša Romčević, Veljko Đokić, Ljiljana Damnjanović, Aleksandar Dekanski, Mira Vukčević.
Conference Secretary: Jasmina Jevtić

Conference Technical Committee

Sonja Jovanović, Ivana Dinić, Željko Mravik, Željko Radovanović, Vukašin Ugrinović, Tamara Matić, Jelena Rmuš, Marija Milivojević, Milica Stefanović, Ivana Banićević, Dušana Nedović.

HISTORY

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).

YUCOMAT 2021 GENERAL INFORMATION

DATE AND VENUE: The conference will be held on August 30 - September 3, 2021, at the **Hunguest Hotel Sun Resort**, in Herceg Novi, Montenegro. Participants will also be accommodated there. The conference will begin on Monday, August 30th, at 09.00 and end on Friday, September 3rd, 2021, at 12.00.

REGISTRATION: Registration, registration fee payment, conference materials distribution, etc, will take place at the conference desk (Conference Secretariat) open on Sunday, August 29, and Monday, August 30, from 8.00 to 19.00, on Tuesday, Wednesday and Thursday 8.00-13.00 and 19.00-20.00, and on Friday from 8.00 to 12.00. At registration, the participants are requested to submit a proof of their advance registration fee payment.

VIRTUAL PRESENTATIONS: The abstracts of the Virtual Presentations are within the abstracts of the Plenary, Oral and Poster Sections in this book. Lectures are located on the YUCOMAT 2021 Conference site: https://www.mrs-serbia.org.rs/index.php/virtual-offline-presentations from August 23, 2021, to 7 days after the deadline for the end of the Conference (September 10, 2021).

INSTRUCTION FOR AUTHORS: The conference will feature Plenary Sessions, Oral Sessions, Poster Sessions, Virtual Offline Session. Time of papers' presentations to be given in Oral Sessions is limited. Time available for delivery is 30 min for plenary and 15 min for other papers, including discussion. Video-beam is available. PowerPoint presentations, recorded on CD or USB flash-memory, should be given at the start of 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 Wednesday.

CONFERENCE AWARDS: Joint Award by MRS-Singapore and MRS-Serbia at the YUCOMAT 2021 Conference. Sponsorship of the ten Awards in the financial amount by the MRS-Singapore, to the authors not older than 35 for the best: Five Oral presentation and Five Posters presentation. Awarded authors will be announced at the Closing Ceremony of the Conference. Each award consists of a financial amount honorarium, diploma, meeting registration fee to attend the next YUCOMAT 2022 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 CONFERENCE PROGRAM

Sunday, August 29, 2021

08.00-19.00 **Registration**

Monday, August 30, 2021

08.00-19.00 **Registration**

09.00-10.30 **OPENING CEREMONY**

- Introduction and Welcome, Main Conference Hall
- **The Laureate of the 2020 MRS-Serbia,** Award for a Lasting and Outstanding Contribution to Materials Science and Engineering
  Robert Sinclair, Virtual lecture
- **The Laureate of the 2021 MRS-Serbia,** Award for a Lasting and Outstanding Contribution to Materials Science and Engineering
  Yury Gogotsi

11.00-12.30 **First Plenary Session**, Main Conference Hall

13.00-13.30 **Photo Session**

15.00-19.00 **Second Plenary Session (Virtual Offline)**, Main Conference Hall

19.30-21.30 **Cocktail Party**

Tuesday, August 31, 2021

08.00-12.45 **First Oral Session,** Main Conference Hall
Competition for the best Oral presentation of young researchers

15.00-18.00 **First Poster Session**, National Restaurant Jadranka Terrace
Competition for the best Poster presentation of young researchers

Wednesday, September 1, 2021

08.00-10.00 **Second Poster Session**, National Restaurant Jadranka Terrace

10.30-13.00 **Third Plenary Session,** Main Conference Hall

15.00-18.00 **Third Poster Session,** National Restaurant Jadranka Terrace

Thursday, September 2, 2021

08.30-13.00 **Second Oral Session**, Main Conference Hall

15.00-19.00 **Boat-trip around Boka Kotorska Bay**

Friday, September 3, 2021

09.00-10.30 **Third Oral Session**, Main Conference Hall

10.30-11.00 **Awards and Closing of the Conference**

11.00 **Cocktail and Greetings for Goodbye to all YUCOMAT participants**

Virtual Presentations

The abstracts of the Virtual Presentations are within the abstracts of the Plenary, Oral and Poster Sections in this book. Presentations can be accessed from the YUCOMAT 2021 Conference site: https://www.mrs-serbia.org.rs/index.php/virtual-offline-presentations, from August 23, 2021, to 7 days after the deadline for the end of the Conference (September 10, 2021).

SCIENTIFIC PROGRAM

Monday, August 30, 2021

Main Conference Hall

OPENING CEREMONY

09.00-09.30 **Welcome Speech**
Dragan Uskoković, President of MRS-Serbia, Belgrade, Serbia

Presentation of YUCOMAT 2019 Awards
Velimir Radmilović, Vice President of MRS-Serbia

09.30-10.00 **MRS-Serbia 2020 Award for a Lasting and Outstanding Contribution to Materials Science and Engineering**
Robert Sinclair, Stanford University, Stanford, CA, USA
In situ High Resolution Electron Microscopy of Material Reactions at the Atomic Level
Virtual Lecture

10.00-10.30 **MRS-Serbia 2021 Award for a Lasting and Outstanding Contribution to Materials Science and Engineering**
Yury Gogotsi, Drexel University, Philadelphia, USA
MXenes - Two-Dimensional Materials for Future Technologies

10.30-11.00 **Break**

FIRST PLENARY SESSION
Main Conference Hall

Session I: 11.00 -12.30
Chairpersons: Hamish Fraser and Ruslan Valiev

11.00-11.30 **The Lithium Battery, from a Dream to a Readiness to Take on Climat Change - Materials Opportunities and Challenges, Virtual lecture**
Michael Stanley Whittingham, *Nobel Laureate in Chemistry 2019 for the development of lithium-ion batteries*
Binghamton University, State University of New York, US

11.30-12.00 **Bulk nanostructured metallic materials with multifunctional properties: innovative applications and challenges in commercialization**
Ruslan Z. Valiev, Ufa State Aviation Technical University, 12 Karl Marx Street, Ufa 450008, Russia; Saint Petersburg Saint Petersburg State University, Saint Petersburg, Russia

12.00-12.30 **Exploiting structural and compositional instabilities in titanium alloys to optimize properties of components fabricated by additive manufacturing**
Hamish Fraser[1], Brian Welk[1], Nevin Taylor[1], Zachary Kloenne[1], Yufeng Zheng[2], Rajarshi Banerjee[3]
[1]The Ohio State University; [2]University of Nevada-Reno; [3]University of North Texas

13.00-13.30 **Photo session**

13.00-15.00 **Break**

Main Conference Hall

SECOND PLENARY SESSION (VIRTUAL OFFLINE)

Session I: 15.00-16.30
Chairpersons: Đorđe Janaćković and Petar Uskoković

15.00-15.30 **Bioinspired Super-wettability System and Beyond Quantum-confined Superfluid: Energy Conversion, Chemical Reaction and Biological Information Transfer**
Lei Jiang, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing, P. R. China

15.30-16.00 **Engineering advanced materials through polyphenol-mediated assembly**
Frank Caruso, ARC Centre of Excellence in Convergent Bio-Nano Science and Technology, and the Department of Chemical Engineering, The University of Melbourne, Parkville, Victoria 3010, Australia

16.00-16.30 **Intelligent Biomaterials**
Seeram Ramakrishna, Center for Nanotechnology & Sustainability, National University of Singapore

16.30-17.00 **Break**

Session II: 17.00-19.00
Chairpersons: Đorđe Janaćković and Petar Uskoković

17.00-17.30 **Engineering human tissues for medical impact**
Gordana Vunjak-Novakovic, The Mikati Foundation Professor of Biomedical Engineering and Medical Sciences, Columbia University in the City of New York

17.30-18.00 **Cluster-assembled materials**
Horst Hahn, Karlsruhe Institute of Technology (KIT), Germany

18.00-18.30 **Stabilization of metastable states for sustainable functionalization -From molecular dispersion to spintronics**
Mamoru Senna, Faculty of Science and Technology, Keio University

18.30-19.00 **Constitution and Structural Chemistry of T-Mn Systems (T = Sc to Ta)**
P. Rogl[1], X. Yan[1], X.Q. Chen[1], P. Broz[2], J. Vrestal[2], J. Bursik[3], J. Pavlu[2], B. Smetana[4], G. Rogl[1], A. Grytsiv[1], H. Michor[5]
[1]Institute of Materials Chemistry, University of Vienna, 1090 Wien, Austria, [2]Department of Chemistry, Faculty of Science, Masaryk University, Brno, Czech Republic, [3]Institute of Physics of Materials, Czech Acad. of Sci., Brno, Czech Republic, [4]Faculty of Materials Science and Technology, VSB-TU Ostrava, Czech Republic, [5]Institute of Solid State Physics, TU-Wien, 1040 Wien, Austria

19.30-21.30 **COCKTAIL PARTY**

Tuesday, August 31, 2021

Main Conference Hall

FIRST ORAL SESSION
Competition for the best Oral presentation of young researchers

Session I: 08.00-10.30
Chairpersons: Bojana Obradović and Zoran Jovanović

08.00-08.15 **Phase Transformations in a Heterogeneous Ti-xNb-7Zr-0.8O Alloy Prepared by a Field-assisted Sintering Technique**
Jiří Kozlík[1], Tomáš Chráska[2], Miloš Janeček[1], Dalibor Preisler[1], Josef Stráský[1], Jozef Veselý[1], Anna Veverková[1]
[1]Charles University, Department of Physics of Materials, Prague, Czechia, [2]Institute of Plasma Physics, Materials Engineering Department, Prague, Czechia

08.15-08.30 **Tuning the thermoelectric performance of $CaMnO_3$-based ceramics by controlled exsolution and micro-structuring**
Nikola Kanas[1,2], Benjamin A. D. Williamson[2], Richard Hinterding[3], Mari-Ann Einarsrud[2], Sverre Magnus Selbach[2], Armin Feldhoff[3], and Kjell Wiik[2]
[1]Institute Biosense, University of Novi Sad, Novi Sad, Serbia, [2]Department of Materials Science and Engineering, NTNU Norwegian University of Science and Technology, Trondheim, Norway, [3]Institute of Physical Chemistry and Electrochemistry, Leibniz University, Hannover, Germany

08.30-08.45 **Low dimensional properties of transition metals with 1H-1,2,4-Triazole**
Shiraz Ahmed Siddiqui[1] , Jana Kalbáčová Vejpravová[2], Hidetsugu, Shiozawa[1,3]
[1]University of Vienna & VDS, Vienna, Austria ,[2]Charles University, Prague, Czech Republic, [3]J. Heyrovsky Institute of Physical Chemistry, Prague, Czech Republic

08.45-09.00 **Odd-Even Effect in Molecular Packing of Self-Assembled Monolayers of Biphenyl-Substituted Fatty Acid on Ag(111)**
A. Krzykawska, J. Ossowski, M. Szwed, P. Cyganik
Department of Physics of Nanostructures and Nanotechnology, Jagiellonian University, Krakow, Poland

09.00-09.15 **An in-situ study on phase transformations in metastable β titanium and zirconium alloys**
A. Veverková, D. Preisler, V. Valešová, P. Harcuba, J. Šmilauerová, J. Strásk
Department of Physics of Materials, Charles University, Ke Karlovu 5, 12116, Prague, Czech Republic

09.15-09.30 **Fronts of the Deformation Phase Transformation in TRIP-steel**
Lidiya Danilova, Dina Orlova, Vladimir Danilov
Institute of Strength Physics and Materials Science SB RAS, Tomsk, Russia

09.30-09.45 **Magneto-optic Janus nanoplatelets**
Jelena Papan[1,2], Patricija Hribar Boštjančič[1,3], Alenka Mertelj[1], Darja Lisjak[1]
[1]Jožef Stefan Institute, Jamova cesta 39, Ljubljana, Slovenia, [2]Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, P.O. Box 522, Belgrade, 11001 Serbia, [3]Jožef Stefan International Postgraduate School, Jamova cesta 39, Ljubljana, Slovenia

09.45-10.00 **Facile Microwave Assisted Synthesis of Silica Based Nanocoatings with Tunable Wettability**
Maria Antonia Tănase[1], Adina Răducan[1], Petruţa Oancea[1], Cătălin Ionuţ, Mihăescu[2], Claudia Ninciuleanu[2], Elvira Alexandrescu[2], Cristina Scomoroscenco[2], Cristian Petcu[2], Ludmila Otilia Cinteză[1]
[1]University of Bucharest, Physical Chemistry Department, 4-12 Elisabeta Blvd, Bucharest, Romania,[2]INCDCP-ICECHIM, Polymer Department, 202 Splaiul Independentei, Bucharest, Romania

10.00 -10.15 **Oscillation in Stability of Consecutive Chemical Bonds in Self – Assembled Monolayers with Carboxylic Binding Group**
Mateusz Wróbel[1], Jakub Ossowski[1], Mariusz Krawiec[2], Krzysztof Kozieł[3], Paweł Dąbczyński[1], Piotr Cyganik[1]
[1]Smoluchowski Institute of Physics, Jagiellonian University, Łojasiewicza 11, 30-348 Kraków, Poland, [2]Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Kraków, Poland, [3]Marie Curie Sklodowska University, Institute of Physics, Pl. M. Curie-Skłodowskiej 1, 20-031 Lublin, Poland

10.15 -10.30 **The Odd-Even Effect in Electron Beam Irradiation of Hybrid Aromatic-Aliphatic Self-Assembled Monolayers of Fatty Acid**
Monika Kruk[1], Christof Neumann[2], Martha Frey[2], Krzysztof Kozieł[3], Andrey Turchanin[2], Piotr Cyganik[1]
[1]Smoluchowski Institute of Physics, Jagiellonian University, 30-348 Krakow, Poland, [2]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany, [3]Faculty of Chemistry, Jagiellonian University, Krakow 30-387, Poland

10.30-11.00 **Break**

Session II: 11.00-12.45
Chairpersons: Bojana Obradović and Zoran Jovanović

11.00-11.15 **Super porous hydrogels based on poly(N-isopropylacrylamide) for potential application as soft actuators with extreme-fast volume responsive temperature- and pH-sensitive properties**
S. Horodecka, K. Hishchak, B. Strachota, A. Strachota, M. Šlouf
Institute of Macromolecular Chemistry, Czech Academy of Sciences, Heyrovského nám. 2, CZ-162 06 Praha 6, Czech Republic

11.15-11.30 **Electrochemical reduction of CO_2 on electrodeposited copper-based nanoparticles: Stability Study**
Stefan Popović[1,2], Marjan Bele[1], Nejc Hodnik[1,2]
[1]Department of Materials Chemistry, National Institute of Chemistry Hajdrihova 19, 1000 Ljubljana, Slovenia ,[2]University of Nova Gorica Vipavska 13, 5000 Nova Gorica, Slovenia

11.30-11.45 **Catalyst Screening for Homogeneous and Heterogeneous Carboxylation of Lignin-derived Model Compounds**
Aleksa Kojčinović, Gorica Ivaniš, Blaž Likozar, Miha Grilc
Department of Catalysis and Chemical Reaction Engineering, National Institute of Chemistry, Hajdrihova 19, 1000 Ljubljana, Slovenia

11.45-12.00 **Novel Magnesium Alloy Mg-4Gd-4Y-2Ca with enhanced ignition temperature and mechanical properties**
Jitka Stráská[1], Jiří Kubásek[2], Peter Minárik[1], Klára Hosová[2], Stanislav Šašek[1], Michal Knapek[1], Jozef Veselý[1], Drahomír Dvorský[2], Dalibor Vojtěch[2]
[1]Charles University, Faculty of Mathematics and Physics, Department of Physics of Materials, Ke Karlovu 5, 121 16 Praha 2, Czech Republic, [2]University of Chemistry and Technology, Faculty of Chemical Technology, Department of Metals and Corrosion Engineering, Technická 5, 166 28 Praha 6, Czech Republic

12.00-12.15 **Properties of belite-calcium sulfoaluminate cements synthesized from various industrial residues**
Katarina Šter, Maruša Borštnar, Sabina Dolenec
Slovenian National Building and Civil Engineering Institute, Dimičeva ulica 12, 1000 Ljubljana, Slovenia

12.15-12.30 **Microkinetic Study of Furfural Hydrotreatment over Various MoO_x-Based Catalysts**
Miha Grilc, Aleksa Kojčinović, Žan Kovačič, Matej Huš, Blaž Likozar
Department of Catalysis and Chemical Reaction Engineering, National Institute of Chemistry, Hajdrihova 19, 1000 Ljubljana, Slovenia

12.30-12.45 **Microstructure and corrosion properties of a novel biomedical WN43 Magnesium alloy prepared by spark plasma sintering**
Mária Zemková[1], František Lukáč[2], Jan Bohlen[3], Robert Král[1], Peter Minárik[1]
[1]Charles University, Prague, Czech Republic; [2]Institute of Plasma Physics, Czech Academy of Science, Prague, Czech Republic; [3]Magnesium Innovation Center, Geesthacht, Germany

12.45-15.00 **Break**

National Restaurant Jadranka Terrace

FIRST POSTER SESSION
Competition for the best Poster presentation of young researchers

Session I: 15.00-18.00
Chairpersons: Smilja Marković and Dragana Jugović

P.S.I.1.
Utilization of nitrogen doped carbon cryogel for efficient removal of pharmaceutical residues from water
Aleksandar Krstić[1], Aleksandar Lolić[2], Miljana Mirković[1], Ana Kalijadis[1]
[1]University of Belgrade, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, Mike Petrovića Alasa 12-14, Belgrade, Serbia, [2]University of Belgrade, Faculty of Chemistry, Studentski trg 12-16, Belgrade, Serbia

P.S.I.2.
Mercerized jute fabrics suitable for technical textiles
Aleksandra Ivanovska[1], Koviljka Asanovic[2], Maja Jankoska[3], Mirjana Kostic[2]
[1]University of Belgrade, Innovation Center of the Faculty of Technology and Metallurgy, Karnegijeva 4, 11000 Belgrade, Serbia, [2]University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11000 Belgrade, Serbia, [3]Ss. Cyril and Methodius University in Skopje, Faculty of Technology and Metallurgy, Ruger Boskovic 16, 1000 Skopje, North Macedonia

P.S.I.3.

Oxygen diffusion in doped Ti-Al alloys

Alexander V. Bakulin[1,2], Ekaterina V. Matyskina[2], Svetlana E. Kulkova[1,2]
[1]ISPMS SB RAS, Tomsk, Russia, [2]TSU, Tomsk, Russia

P.S.I.4.

Mechanochemical synthesis of TiO_2-CeO_2 powder for the purpose of building an oxygen sensor

Jelena N Stevanović[1], Srđan Petrović[1], Marko V Bošković[1], Dana Vasiljević Radović[1], Ivana O. Mladenović[1], Biljana Šljukić[2,3], Milija Sarajlić[1]
[1]Institute of Chemistry, Technology and Metallurgy, Njegoševa 12, Belgrade, Serbia, [2]Faculty of Physical Chemistry, Studentski trg 12-16, University of Belgrade, Belgrade, Serbia, [3]CeFEMA, Instituto Superior Téchnico, Universidade de Lisboa, 1049-001 Lisbon, Portugal

P.S.I.5.

Understanding the photopolymerization and post-processing as a way to enhance thermomechanical properties of 3D printed auxetic structures

Martina Štaffová, František Ondreáš
Central European Institute of Technology, Brno, University of Technology, Purkynova 656/123, Brno 612 00, Czech Republic

P.S.I.6.

Stability of Pt-based alloy ORR electrocatalysts for PEM fuel cells: Temperature dependent metal dissolution

Tina Đukić, Léonard Jean Moriau, Martin Šala, Luka Pavko, Mitja Kostelec, Matija Gatalo, Nejc Hodnik
National Institute of Chemistry, Hajdrihova 19, 1000 Ljubljana, Slovenia

P.S.I.7.

High entropy materials for electrochemical applications

David Stenze, Abhishek Sarkar, Qingsong Wang, Horst Hahn, Ben Breitung
Karlsruhe Institute of Technology, Institute of Nanotechnology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

P.S.I.8.

Resistive Switching Memory Devices based on 2D Halide Perovskites

Hyojung Kim, Ho won Jang
Department of Materials Science and Engineering, Seoul National University, Seoul, South Korea

P.S.I.9.

Electrochemical control of magnetism: on the conversion of hydrated FeF_3 with Li to Fe and LiF

Ruby Singh[1,2], Ralf Witte1, Xiaoke Mu[1,3], Torsten Brezesinski[1], Ben Breitung[1,2], Robert Kruk[1], Horst Hahn[1,2]
[1]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), 76344 Eggenstein-Leopoldshafen, Germany, [2]Joint Research Laboratory Nanomaterials, Technische Universität Darmstadt & Karlsruhe Institute of Technology (KIT), 64287 Darmstadt, Germany, [3]Karlsruhe Nano-Micro Facility (KNMF), Karlsruhe Institute of Technology (KIT), 76344 Eggenstein-Leopoldshafen, Germany

P.S.I.10.

Electrical properties of epoxy composites based on carbon black and multi- walled carbon nanotubes

Artyom A. Shestakov[1], Alexander G. Bannov[1], Andrey E. Brester[1], Nikita I. Lapekin[1], Arina V. Ukhina[2], Evgeniy A. Maksimovskii[1,3]
[1]Novosibirsk State Technical University, Novosibirsk, 630073, Russia, [2]Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk, 630128, Russia, [3]Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk, 63009, Russia

P.S.I.11.

Increasing catalytic activity of molybdenum disulfide for hydrogen evolution reaction

Jelena Rmuš[1], Anđela Mitrović[1], Ana Mraković[2], Željko Mravik[1], Tijana Pantić[1], Ivana Stojković Simatović[3], Sandra Kurko[1]

[1]Center of excellence for hydrogen and renewable energy (CONVINCE), Department of Physics, "Vinča" Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia, [2]Department of Theoretical Physics and Condensed Matter Physics, "Vinča" Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia, [3]Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia

P.S.I.12.

Investigation of thermodynamic parameters of high concentration alkaline activators in the geopolymerization process of metakaolin

Marija Ivanović[1], Snežana Nenadović[1], Nataša Mladenović Nikolić[2], Miljana Mirković[1], Ljiljana Kljajević[1]

[1]Department of Materials Science, Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia University of Belgrade, Serbia, [2]Department of Nuclear and Plasma Physics, Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, Serbia

P.S.1.13.

Morphology and mechanical properties of the nanotubular oxide coating formed on the ultra-fine-grained Ti-13Nb-13Zr alloy

Dragana R. Barjaktarević, Veljko R. Đokić, Đorđe N. Veljović, Marko P. Rakin

[1]University of Belgrade, Faculty of Technology and Metallurgy, 11120 Belgrade, Serbia

P.S.I.14.

Optimization of in vitro conditions for 3D culture of rat glioma cells

Jelena Petrović[1,2], Mia Radonjić[1,2], Jasmina Stojkovska[1,2], Bojana Obradovic[1]

[1]Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, [2]Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia

P.S.I.15.

A Possible Approach in Wound Management – An Exfoliated Hydrogel Layer, Based On Polysaccharide Gum Karaya Modified With Carboxymethyl Cellulose, Covered by Natural Hydrophobic Layer

Katarína Kacvinská[1], Lucy Vojtová[1], Petr Poláček[1], Šárka Kobzová[2], Lubomír Janda[2], Petr Sedláček[3]

[1]CEITEC-Central European Institute of Technology, Advanced Biomaterials, Purkyňova 656/123, 612 00 Brno Brno, Czech Republic; [2]Veterinary Research Institute, Hudcova 296/70, 621 00 Brno, Czech Republic; [3]Brno Univ. of Technol., Purkyňova 464/118, Královo Pole, 61200, Brno, Czech Republic

P.S.I.16.

Pro-healing protein release from 3D-printed „smart“ hydrogel carriers applicable in regenerative medicine

Klára Lysáková[1], Kristýna Valová[1], Nikola Křivánková[1], Lucy Vojtová[1]

[1]Brno University of Technology, CEITEC-Central European Institute of Technology, Advanced Biomaterials, Purkyňova 656/123, 612 00 Brno, Czech Republic

P.S.I.17.

Viscoelastic properties of resorbable PLGA-PEG-PLGA based bioinks for additive manufacturing technology in regenerative medicine

Kristýna Valová, Klára Lysáková, Nikola Křivánková, Lucy Vojtová

Brno University of Technology, CEITEC-Central European Institute of Technology, Advanced Biomaterials, Purkyňova 656/123, 612 00 Brno, Czech Republic

P.S.I.18.

Synthesis, characterization and possible application of bacterial cellulose-ceria composite

Svetlana Butulija[1], Jelena Filipović Tričković[1], Ana Valenta[1], Željko Radovanović[2], Bojana Ćetenović[1], Danica Zmejkoski[1], Bratislav Todorović[3], Branko Matović[1]

[1]Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia, [2]Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia, [3]Faculty of Technology, University of Niš, Leskovac, Serbia

P.S.I.19.

Hydroxyapatite based inserts in restorative dentistry: Effects of calcium substitutions on the bonding ability

Tamara Matić[1], Maja Ležaja Zebić[2], Vesna Miletić[2], Rada Petrović[3], Đorđe Janaćković[3], Đorđe Veljović[3]

[1]University of Belgrade, Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia, [2]University of Belgrade, School of Dental Medicine, Belgrade, Serbia, [3]University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia

P.S.I.20.

Poly (methacrylic acid)/gelatin/hydroxyapatite composite hydrogels for bone tissue engineering

Vukašin Ugrinović[1], Bojan Božić[2], Rada Petrović[3], Đorđe Janaćković[3], Đorđe Veljović[3]

Innovation Center of Faculty of Technology and Metallurgy, Belgrade, Serbia, [2]Institute of Physiology and Biochemistry „Ivan Đaja“, Faculty of Biology, Belgrade, Serbia, [3]Department of Inorganic Chemical Technology, Faculty of Technology and Metallurgy, Belgrade, Serbia

P.S.I.21.

Wettability of polysiloxane-CNTs composite coatings deposited on glass supports activated by cold plasma

Michał Chodkowski[1], Iryna Sulym[2], Konrad Terpiłowski[1]

[1]Department of Interfacial Phenomena, Institute of Chemical Sciences, Faculty of Chemistry, Maria Curie-Skłodowska University in Lublin (UMCS) pl. Marii Curie-Skłodowskiej 3, 20-031 Lublin, Poland. [2]Laboratory of Oxide Nanocomposites, Chuiko Institute of Surface Chemistry, NASU, 17 General Naumov Str., 03164 Kyiv, Ukraine.

P.S.I.22.

Compacted carbon nanomaterials and their conductivity

Nikita I. Lapekin, Artyom A. Shestakov, Andrey E. Brester, Alexander G. Bannov

Novosibirsk State Technical University, 630073, Novosibirsk, Russian Federation

Wednesday, September 1, 2021

National Restaurant Jadranka Terrace

SECOND POSTER SESSION

Session I: 08.00-10.00
Chairperson: Sonja Jovanović and Đorđe Veljović

P.S.II.1.

Structural characterization of TiO_2/CNTs nanocomposites aimed for incorporation in facial masks

Anita Grozdanov, Perica Paunovic

Faculty of Technology and Metallurgy, University Ss Cyril and Methodius in Skopje, Rugjer Boskovic 16, 1000 Skopje, North Macedonia

P.S.II.2.

Densification of boron carbide under high pressures and temperatures

Branko Matović

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

P.S.II.3.

Detection of Glyphosate by Surface-Enhanced Raman Spectroscopy

L. Mikac[1,2], M. Gotić[1,2], I. Rigó[3], M. Veres[3], M. Ivanda[1,2]

[1]Center of Excellence for Advanced Materials and Sensing Devices, Ruđer Bošković Institute, Bijenička c. 54, Zagreb, Croatia, [2]Molecular Physics and New Materials Synthesis Laboratory, Ruđer Bošković Institute, Bijenička 54, 10000 Zagreb, Croatia, [3]Department of Applied and Nonlinear Optics, Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Budapest, Hungary

P.S.II.4.

High Torsion Pressure effect on cast and wrought technical grade pure magnesium

Pavel Doležal[1], Jakub Poloprudský[1,2], Jan Čupera[1]

[1]Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czech Republic, [2]Institute of Physics of Materials Czech Academy of Sciences, Brno, Czech Republic

P.S.II.5.

Highly hydrophobic self-assembled monolayers on aluminium – carboxylate vs. phosphonate

Daria M. Cegiełka and Piotr Cyganik

Smoluchowski Institute of Physics, Jagiellonian University, Łojasiewicza 11, 30-348 Kraków, Poland

P.S.II.6.

Degradation of textile dyes by Oxone® activated by cobalt supported chitosan-derived carbon-smectite catalyst

G. Stevanović, N. Jović-Jovičić, B. Dojčinović, A. Milutinović-Nikolić, S. Marinović, P. Banković, M. Ajduković

Institute of Chemistry, Technology and Metallurgy, National Institute, Njegoševa 12, University of Belgrade, Serbia

P.S.II.7.

Spectroscopic characterization and redox behaviour of electroconducting poly(p-ADPA) synthesized by simple and eco-friendly method using magnetite nanoparticles as a catalyst

Jana Mišurović[1], Budimir Marjanović[2], Gordana Ćirić-Marjanović[3]

[1]University of Montenegro-Faculty of Metallurgy and Technology, Cetinjski put bb, 81000 Podgorica, Montenegro, [2]Centrohem, Vuka Karadžića bb, 22300 Stara Pazova, Serbia, [3]University of Belgrade-Faculty of Physical Chemistry, Studentski Trg 12–16, 11158 Belgrade, Serbia

P.S.II.8.

Magnetic characteristics of nanocrystalline electrodeposit of $Ni_{86.0}Fe_{9.8}W_{1.3}Cu_{1.9}$

Milica Spasojević[1], Milan Plazinić[2], Nemanja Stojanović[2], Milentije Luković[2], Aleksa Maričić[2], Miroslav Spasojević [2]

[1]Innovation Center of the Faculty of Chemistry, University of Belgrade, Belgrade, Serbia, [2]Joint Laboratory for Advanced Materials of SASA, Section for Amorphous Systems, Faculty of Technical Sciences, Čačak, University of Kragujevac, Čačak, Serbia

P.S.II.9.

The effect of grinding time, pressing and sintering of the powders 16% Fe_2O_3, 4%$BaCO_3$, 80%$BaTiO_3$ on the morphology, microstructure, magnetic and electrical properties

Milentije Luković[1], Milica Spasojević[2], Suzana Arnaut[1], Slobodan Đukić[1], Siniša Ranđić[1]
[1]Joint Laboratory for Advanced Materials of SASA, Section for Amorphous Systems, Faculty of Technical Sciences, Čačak, University of Kragujevac, Čačak, Serbia, [2]Innovation Center of the Faculty of Chemistry, University of Belgrade, Belgrade, Serbia

P.S.II.10.

Frequency behavior of Co-based amorphous wire MI-element

Jelena Orelj[1], Nebojša Mitrović[1], Vladimir Pavlović [2]
[1] Faculty of Technical Sciences Čačak, University of Kragujevac, Joint Laboratory of Advanced Materials of Serbian Academy of Sciences and Arts, Svetog Save 65, 32 000, Čačak, Serbia, [2]Institute of Technical Sciences of Serbian Academy of Sciences and Arts, Knez Mihailova 35, 11 000, Belgrade, Serbia

P.S.II.11.

Luminescence response of YAP:Mn crystal to the ionizing and visible radiation

Oleksandr Poshyvak[1], Denis Afanassyev[1],Sergii Ubizskii[1],Andriy Luchechko[2]
[1]Lviv Polytechnic National University, [2]Ivan Franko National University of Lviv

P.S.II.12.

Activated Carbon Derived from Vine Shoots as Electrode Material for High-Performance Supercapacitors

Veselinka Grudić[1], Aleksandra Gezović[1], Jana Mišurović[1], Jugoslav Krstić[2], Milica Vujković[3]
[1]Faculty of Metallurgy and Technology, University of Montenegro, Cetinjski put bb, 81000 Podgorica, Montenegro, [2]Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 12, Belgrade, Serbia, [3]Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12–16, 11158 Belgrade, Serbia

P.S.II.13.

X-ray properties spectroscopy and electron structure of $Ca_3Ga_2Ge_4O_{14}$ garnet with dopped Ce (Eu)

Ivan Shcherba[1], Lyudmyla Kostyk[1], Henryk Noga[2], Dragan Uskokovic[3], Lev Bekenov[4], Vitalij Denys[1]
[1]The Ivan Franko National University of Lviv, Kyryla & Metodiya Str. 8, 79-005 Lviv, Ukraine, [2]Institute of Technology, the Pedagogical University of Cracow, Podchorazych Str. 2 Cracow 30-084 Poland,[3]Institute of Technical Sciences of SASA Knez Mihailova 35/IV, PO Box 377, 11000 Belgrade, Serbia, [4]G. V. Kurdyumov Institute for Metal Physics of the N.A.S.U. Kyiv, Ukraine

P.S.II.14.

Sol-gel based synthesis and magnetic, dielectric and optical properties study of nanocrystalline $Sr_3Co_2WO_9$ triple perovskite

Igor Djerdj[1], Jelena Bijelić[1], Martina Medvidović-Kosanović[1], Pascal Cop[2], Ákos Kukovecz[3], Zvonko Jagličić[4], Sugato Hajra[5], Bernd M. Smarsly[2]
[1]Josip Juraj Strossmayer University of Osijek, Department of Chemistry, Cara Hadrijana 8/A, 31000 Osijek, Croatia, [2]Justus-Liebig-Universität, Physikalisch-Chemisches Institut, Heinrich-Buff-Ring 17, D-35392 Gießen, Germany, [3]University of Szeged, Interdisciplinary Excellence Centre, Department of Applied and Environmental Chemistry, Rerrich Bélatér 1, H-6720 Szeged, Hungary, [4]University of Ljubljana, Faculty of Civil and Geodetic Engineering, Jamova 2, SI-1000 Ljubljana, Slovenia, [5]Institute of Technical Education and Research Siksha O Anusandhan (Deemed to be University), 751030 Bhubaneswar, India

P.S.II.15.

Sonochemical synthesis of up-converting β-NaYF$_4$: Yb, Er nanoparticles

Ivana Dinić[1], Marina Vuković[2], Paula Mendes Jardim[3], Marko Nikolić[4], Lidija Mančić[1]
[1]Institute of Technical Sciences of SASA, Belgrade, Serbia, [2]Innovative Centre Faculty of Chemistry Belgrade, University of Belgrade, Serbia, [3]Department of Metallurgical and Materials Engineering, Federal University of Rio de Janeiro, Brazil, [4]Photonic Center, Institute of Physics Belgrade, University of Belgrade, Serbia

P.S.II.16.

Optoelectronic Processes through Molecular Nanofilms

Jovan P. Šetrajčić[1], Stevo K. Jaćimovski[2], Siniša M. Vučenović[1,3], Ana J. Šetrajčić–Tomić[1], Nikola R. Vojnović[4], Igor J. Šetrajčić[1]
[1]Academy of Sciences and Arts of the Republic of Srpska, Banja Luka, Republic of Srpska – B&H, [2]University of Criminal Investigation and Police Studies, Zemun, Vojvodina – Serbia, [3]University of Banja Luka, Faculty of Sciences, Banja Luka, Republic of Srpska – B&H, [4]University of Novi Sad, Faculty of Technical Sciences, Novi Sad, Vojvodina – Serbia

P.S.II.17.

History and new trends in nanoSPD-related research

Zarema Safargalina, Lyubov Egorova, Igor A. Alexandrov
Institute of Physics of Advanced Materials, Ufa State Aviation Technical University, Ufa, 450008, Russia

P.S.II.18.

Anisotropic iron oxide nanostructures with potential applications in biomedicine

Marin Tadic[1], Lazar Kopanja[2,3], Biljana Vucetic Tadic[4], Slavko Kralj[5]
[1]Condensed Matter Physics Laboratory, Vinca Institute of Nuclear Science, University of Belgrade, POB 522, 11001 Belgrade, Serbia, [2]Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, PO Box 3503, 11120 Belgrade, Serbia, [3]Faculty of Mathematics and Computer Science, Alfa BK University, Palmira Toljatija 3, 11070 Belgrade, Serbia, [4]Institute for Mother and Child Healthcare of Serbia, Belgrade, Serbia, [5]Jozef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia

P.S.II.19.

The influence of heteroatoms on physicochemical properties of cobalt ferrite nanoparticles

Sonja Jovanović[1,2], Marija Vukomanović[2], Matjaž Spreitzer[2], Zoran Jovanović[1], Marjeta Maček-Kržmanc[2], Davide Peddis[3,4]
[1]Laboratory of Physics, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia, [2]Advanced Materials Department, Jožef Stefan Institute, Ljubljana, Slovenia, [3]nM2-Lab, Istituto di Struttura della Materia, CNR, Monterotondo Scalo (Roma) 00015, Italy, [4]Department of Chemistry and Industrial Chemistry, University of Genova, Genova, Italy

P.S.II.20.

Journey to the Center of a Perovskite Solar Cell

Vuk V. Radmilović[1], Yi Hou[2], Christoph J. Brabec[2], Erdmann Spiecker[3], Velimir R. Radmilović[4]
[1]Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia, [2]Institute of Materials for Electronics and Energy Technology, Friedrich-Alexander-University Erlangen- Nuremberg, Erlangen, Germany, [3]Center for Nanoanalysis and Electron Microscopy, Friedrich –Alexander -University of Erlangen-Nuremberg, Germany, [4]Serbian Academy of Sciences and Arts, Belgrade, Serbia

10.00-10.30 **Break**
Main Conference Hall

THIRD PLENARY SESSION

Session II: 10.30-13.00
Chairpersons: Velimir Radmilović and Arben Merkoçi

10.30-11.00 **Two-dimensional empty space and its unique properties**
Sir Andre K. Geim, *Nobel Laureate in Physics 2010 for his work on graphene*
University of Manchester, United Kingdom

11.00-11.30 **Advances in molecular beam epitaxy of superconducting materials, Virtual Lecture**
Ivan Bozovic, Brookhaven National Laboratory, Department of Chemistry,
NY and Yale University Connecticut, USA

11.30-12.00 **Nanobiosensors for diagnostics applications**
Arben Merkoçi, Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and The Barcelona Institute of Science and Technology, Campus UAB, Bellaterra, 08193 Barcelona, Spain. ICREA - Institucio Catalana de Recerca i Estudis Avançats, Barcelona, Spain

12.00-12.30 **The "Chemistree" of Porous Solids**
Michael Zaworotko, Department of Chemical Sciences and Bernal Institute, University of Limerick, Ireland

12.30-15.00 **Break**

National Restaurant Jadranka Terrace

THIRD POSTER SESSION

Session III: 15^{00}-18^{00}
Chairpersons: Irena Nikolić and Branko Matović

P.S.III.1.
Thermodynamic characteristics of graphene
S. Jaćimovski[1], D. Raković[2]
[1]Academy of Criminalistic and Police Studies, Belgrade, Serbia, [2] University of Belgrade, Faculty of Electrical Engineering, Serbia

P.S.III.2.
Ion beam irradiation of 12-tungstophosphoric acid – influence of energy of accelerated ions on structural properties
Željko Mravik[1], Danica Bajuk-Bogdanović[2], Andrzej Olejniczak[3,4], Milica Pejčić[2], Jasmina Lazarević[5], Nenad Lazarević[5], Zoran Jovanović[1]
[1]Center of excellence for hydrogen and renewable energy (CONVINCE), Department of Physics, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia, [2]Faculty of Physical Chemistry, University of Belgrade, P.O. Box 47, 11158 Belgrade, Serbia, [3]Flerov Laboratory of Nuclear Reactions, Joint Institute for Nuclear Research, 141980 Dubna, Moscow region, Russia, [4]Faculty of Chemistry, Nicolaus Copernicus University, Toruń, Poland, [5]Center for Solid State Physics and New Materials, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, Belgrade 11080, Serbia

P.S.III.3.

Synthesis and deposition of MAPbBr$_3$ perovskite on titania nanotube arrays

Milica Stefanović[1], Jelena Vujančević[2], Rada Petrović[3], Đorđe Janaćković[3]

[1]University of Belgrade, Innovation Center of Faculty of Technology and Metallurgy, Belgrade, Serbia, [2]Institute of Technical Sciences of SASA, 11000, Belgrade, Serbia, [3]University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia

P.S.III.4.

Application of biomass pyrolysis to obtain biofuels

Dajana Savić[1], Vesna Antić[1], Mališa Antić[1] and Branimir Jovančićević[2]

[1]University in Belgrade, Faculty of Agriculture, Nemanjina 6, 11080, Belgrade, Serbia, [2]University of Belgrade, Faculty of Chemistry, Studentski trg 12-16. 11001 Belgrade, Serbia

P.S.III.5.

Solubility of hydrogen in biomass-derived compounds relevant for hydrodeoxygenation process

Gorica Ivaniš, Ljudmila Fele Žilnik, Blaž Likozar, Miha Grilc

Department of Catalysis and Chemical Reaction Engineering, National Institute of Chemistry, Hajdrihova 19, SI-1000 Ljubljana, Slovenia

P.S.III.6.

New environmentally acceptable materials based on flay ash, steelmaking slag and Zn-reach electric arc furnace dust

Irena Nikolić[1], Dijana Đurović[2], Smilja Marković[3], Ljiljana Veselinović[3], Ivona Janković-Častvan[4], Vuk Radmilović[4], Velimir Radmilović[5]

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P.S.III.7.

Effect of filler type on the physico-chemical and mechanical properties of metakaolin-based geopolymer composites

Ljiljana Kljajević[1], Marija Ivanović[1], Miljana Mirković[1], Miloš Nenadović[2], Mira Vukčević[3], Ivana Bošković[3], Snežana Nenadović[1]

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P.S.III.8.

Synthesis and characterization of Schiff-base containing Metal-organic frameworks

Nikola Radnović[1], Chris Hawes[2], Marko Rodić[1], Mirjana Radanović[1], Berta Barta Holló[1], Branko Kordić[1], Srđan Rakić[1], Branislav Jović[1], Jelena Tričković[1]

[1]University of Novi Sad, Faculty of Sciences, Novi Sad, Serbia, [2]Keele University, School of Chemical and Physical Sciences, Keele, United Kingdom

P.S.III.9.

PVC Composites Reinforced by Metallurgical Waste from Ferro-Nickel Industry

Perica Paunovic, Anita Grozdanov

Faculty of Technology and Metallurgy, University Ss Cyril and Methodius in Skopje, Rugjer Boskovic 16, 1000 Skopje, North Macedonia

P.S.III.10.

Effect of temperature and relative humidity on NO_x reaction with $CaCO_3$: competition between nitrite/nitrate formation on filter sheets

Nemanja Barać[1], Patrick Gane[2,3], Katarina Dimić-Mišić[2], Imani Monireh[2], Đorđe Janaćković[3], Petar Usković[3], Ernest Barceló[2,4]

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P.S.III.11.

Functionalization of polycaprolactone fibers by addition of yarrow extract powder

Anđela N. Radisavljević[1], Marija Jovanović[2], Dušica Stojanović[2], Ivana Radović[3], Vesna Radojević[2], Petar Usković[2], Mirjana Rajilić-Stojanović[2]

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P.S.III.12.

Citric acid, polyethylene glycol, and hydroxypropyl methylcellulose as modifiers of doped calcium phosphate cement properties

Tamara Vlajić[1], Đorđe Veljović[2], Aleksa Milovanović[3], Vesna Miletić[1]

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P.S.III.13.

Effect of Nb, Zr and Ta content on properties of Ti-Nb-Ta-Zr-O

Kristián Šalata[1], Dalibor Preisler[1], Lucie Bodnárová[2], Kristýna Halmešová[3], Petr Harcuba[1], Miloš Janeček[1], Josef Stráský[1]

[1]Department of Physics of Materials, Charles University, Prague, Czech Republic, [2]Institute of Thermomechanics, Czech Academy of Sciences, Prague, Czech Republic, [3]Comtes FHT, a.s., Dobřany, Czech Republic

P.S.III.14.

3D printed mucoadhesive gelatin based buccal films

Marija N. Jovanović[1], Anđela N. Radisavljević[2], Miloš M. Petrović[3], Dušica B. Stojanović[1], Svetlana R. Ibrić[4], Petar S. Usković[1]

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P.S.III.15.

Improvement of bioactivity, biocompatibility, and antibacterial properties of titanium scaffold by coating with bioactive glasses and Ag-doped HAP

Marija Milivojević[1], Željko Radovanović[1], Suzana Dimitrijević[2], Rada Petrović[2], Danica Marković[3], Đorđe Janaćković[2]
[1]Innovation Center of Faculty of Technology and Metallurgy, [2]Faculty of Technology and Metallurgy University of Belgrade, [3]Faculty of Veterinary Medicine University of Belgrade

P.S.III.16.

Modelling of catalytic activity and enzyme-MOF interactions using combined *in silico* approach

Milan Senćanski[1], Radivoje Prodanović[2], Predrag Ristić[2], Ana Marija Balaž[3], Marija Stanišić[2], Tamara Todorović[2]
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P.S.III.17.

Synthesis and characterization of Zn(II) and Bi(III) complexes with N-substituted glycine hydrazones

Nevena Stevanović[1], Snežana Selaković[1], Temiloluwa Adejumo[2], Maja Šumar-Ristović[2], Božidar Čobeljić[2], Katarina Anđelković[2]
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P.S.III.18.

Promising Hydroxyapatite/Nifuroksazid Conjugate

Željko Radovanović[1], Katarina Mihajlovski[2], Lidija Radovanović[1], Rada Petrović[2], Đorđe Janaćković[2]
[1]University of Belgrade, Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia, [2]University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia

P.S.III.19.

New biomaterials with Saccharide components. III. The influence of trehaloses on cell membrane enzyme activity and some application in vaccine production

M. M. Plavšić[1,2], D. S. Savić[1], S. R. Savić[1], M. B. Plavšić[3]
[1]University of Niš, Faculty of Technology, Leskovac,[2]The Academy of Applied Technical Studies Belgrade, [3]Belgrade University

P.S.III.20.

Electrospun composite nanofibers containing biocompatible inorganic tungsten disulfide nanoparticles

Dušica B. Stojanović[1], Sergej Tomić[2], Marina Bekić[2], Snežana Zečević[3], Darinka Popović[3], Miodrag Čolić[3], Petar S. Uskoković[1]
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Thursday, September 2, 2021

Main Conference Hall

SECOND ORAL SESSION

Session I: 08.30-13.00
Chairpersons: Milan Stojanović and Konrad Terpiłowski

08.30-08.45 **Are high-entropy alloys better than conventional ones?**
E. Babić[1], Đ. Drobac[2], I. A. Figueroa[3], M. Laurent-Brocq[4], Ž. Marohnić[2], S. Michalik[5], V. Mikšić-Trontl[2], L. Perriere[4], P. Pervan[2], R. Ristić[6], K. Zadro[1]
[1]Department of Physics, Faculty of Science, University of Zagreb, Zagreb, Croatia, [2]Institute of Physics, Bijenička cesta 46, Zagreb, Croatia, [3]Institute for Materials Research-UNAM, Mexico D.F., Mexico, [4]Univrsite Paris Est, ICMPE, F-94320 Thiais, France, [5]Diamond Light Source Ltd., Didcot OX11ODE, UK, [6]Department of Physics, University of Osijek, Osijek, Croatia

08.45-09.00 **Photocatalytic and Photoelectrocatalytic Degradation of Organic Compounds in TiO_2-nanotubes-based Reactors**
Luka Suhadolnik[1], Živa Marinko[1,2], Miran Čeh[1,3]
[1]Nanostructured Materials, Jozef Stefan Institute, Ljubljana, Slovenia,[2]Jozef Stefan International Postgraduate School, Ljubljana, Slovenia, [3]Center for Electron Microscopy and Microanalysis, Jozef Stefan Institute, Ljubljana, Slovenia

09.00-09.15 **Self-organization of plasma in DC and RF magnetron sputtering**
Matjaž Panjan
Jožef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia

09.15-09.30 **PLD growth of functional oxides on graphene oxide-buffered silicon surface**
Zoran Jovanović[1,2], Urška Trstenjak[1], Binbin Chen[3], Elena Tchernychova[4], Matejka Podlogar[5], Gertjan Koster[3], Matjaž Spreitzer[1]
[1]Advanced Materials Department, Jožef Stefan Institute, Ljubljana, Slovenia, [2]Laboratory of Physics, Vinča Institute of Nuclear Sciences, Belgrade, Serbia, [3]MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands, [4]National Institute of Chemistry, Ljubljana, Slovenia, [5]Department for nanostructured materials, Jožef Stefan Institute, Ljubljana, Slovenia

09.30-09.45 **Deposition of metal hydride films by hydrogen transport via a hollow cathode discharge**
Stephen Muhl[1], Argelia Perez[2]
[1]Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, CDMX, México, [2]Unidad de Investigación y Desarrollo Tecnológico (UIDT-CCADET), Hospital General de México, CDMX, México

09.45-10.00 **Combustion synthesis of multilayer Ti–Ta–Ni–Ceramic Composite**
Olga K. Kamynina, S. G. Vadchenko, N. F. Shkodich, I. D. Kovalev
ISMAN, Chernogolovka, Russia

10.00-10.15 **Reversible intercalation/deintercalation of lithium ions within γ-LiV_2O_5 polymorph**
Miloš Milović[1], Milica Vujković[2], Dragana Jugović[1], Miodrag Mitrić[3]
[1]Institute of Technical Sciences of SASA, 11 000 Belgrade, Serbia, [2]Faculty of Physical Chemistry, University of Belgrade, 11 000 Belgrade, Serbia, [3]Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, 11 000 Belgrade, Serbia

10.15-10.30 **TRIP/TWIP effect in beta Ti alloys with high oxygen content**
Josef Stráský, Dalibor Preisler, Michal Knapek, Jiří Kozlík, Petr Harcuba
Department of Physics of Materials, Charles University, KeKarlovu 5, 121 16 Prague, Czech Republic

10.30-11.00 **Break**

11.00-11.15 **Non-oxidative dehydrogenation of propane on chromium(III) oxide: an ab initio study of reaction kinetics and catalyst deactivation**
Matej Huš, Drejc Kopač, Blaž Likozar
National Institute of Chemistry, Department of Catalysis and Chemical Reaction Engineering, Hajdrihova 19, SI-1001 Ljubljana, Slovenia

~~11.15-11.30~~ **Correlation between the evolution of precipitates and microhardness in Inconel 625 fabricated by laser powder bed fusion - transferred to Virtual Offline Presentations**
Kewin Gola, Beata Dubiel, Izabela Kalemba-Rec
AGH University of Science and Technology, Faculty of Metals Engineering and Industrial Computer Science, Cracow, Poland

11.15-11.30 **Thin and Thermally Stable SAMs for Frmation of Higly Conductive or Higly Insulating Organic Monolayers on Metals**
Mateusz Wróbel[1], Anna Krzykawska[1], Eric Sauter Eric[2], Mariusz Krawiec[3], Krzysztof Kozieł[4], Michael Zharnikov[2], Piotr Cyganik[1]
[1]Smoluchowski Institute of Physics, Jagiellonian University, Łojasiewicza 11, 30-348 Kraków, Poland, [2]Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany, [3]Institute of Physics, Maria Curie-Skłodowska University, Pl. M. Curie Skłodowskiej 1, 20-031 Lublin, Poland, [4]Faculty of Chemistry, Jagiellonian University, 30-387 Krakow, Poland

11.30-11.45 **Porous monolithic 3D nanostructures and nanocomposites based on alumina hydroxides**
Anatole. N. Khodan[1], A. Kanaev[2], R. Sh. Askhadullin[3], A. A. Osipov[3], A. A. Angeluts[4], A. A. Konovko[4]
[1]Frumkin Institute for Phisical Chemictry end Electrochemistry RAS, Moscow, Russia, [2]Laboratoire des Sciences des Procédés et des Matériaux CNRS, Villetaneuse, France, [3]Leypunsky Institute for Physics and Power Engineering - IPPE JSC, Obninsk, Russia, [4]Faculty of Physics, Lomonosov Moscow State University, Moscow, Russia

11.45-12.00 **Ordered structures formation in multicomponent polysaccharide systems; effect of graphene oxide**
Ivan Kelnar, Alexander Zhigunov, Sabina Krejčíková, Jiří Dybal
Institute of Macromolecular Chemistry, Czech Academy of Sciences, Heyrovského nám. 2, 162 06 Praha, Czech Republic

12.00-12.15 **ZnO nanoparticles with optimized surface-to-bulk defect ratio for potential biomedical application**
S. Marković,[1] A. Stanković,[1] I. Drvenica,[2] B. Ristić,[3] S.D. Škapin[4]
[1]Institute of Technical Sciences of SASA, Belgrade, Serbia, [2]Institute for Medical Research, University of Belgrade, Belgrade, Serbia, [3]Institute of Microbiology and Immunology, Faculty of Medicine, University of Belgrade, Belgrade, Serbia, [4]Jožef Stefan Institute, Ljubljana, Slovenia

12.15-12.30 **Identical Location Transmission Electron Microscopy Coupled with Modified Floating Electrode Characterisation of Pt-Co/C Electrocatalyst for Oxygen Reduction Reaction**
Armin Hrnjić[1,2], Ana-Rebeka Kamšek[1], Andraž Pavlišič[3], Fransicso Ruiz-Zapeda[1], Matija Gatalo[1], Leonard Moriau[1], Primož Jovanovič[1], Nejc Hodnik[1,2]
[1]Department for Materials Chemistry, National Institute of Chemistry, Hajdrihova 19, SI-1000 Ljubljana, Slovenia, [2]University of Nova Gorica, Vipavska 13, 5000 Nova Gorica, Slovenia, [3]Department of Catalysis and Chemical Reaction Engineering, National Institute of Chemistry, Hajdrihova 19, 1000 Ljubljana, Slovenia

12.30-12.45 **Aptamers on Surfaces: Making of Perfect Bioreceptors for Sensors**
Milan N. Stojanović
Columbia University, Departments of Medicine, and Bioengineering and Systems Biology

Friday, September 3, 2021

Main Conference Hall

THIRD ORAL SESSION

Session I: 09.00-10.30
Chairpersons: Vilma Bursikova and Waldemar Swiderski

09.00-09.15 **Deposition of nanocomposite diamond-like carbon films under dusty plasma conditions**
Vilma Bursikova[1], Štěpánka Bittnerová[1], Roman Přibyl[1], Richard Václavik[1], Monika Stupavská[1], Pavel Sťahel[1], Anna Charvatova Campbell[2], Marek Havlíček[2,3], Petr Klapetek[2], Romana Mikšová[4], Vratislav Perina[4]
[1]Institute of Physical Electronics, Faculty of Science, Masaryk University, Kotlarska 2, CZ-611 37 Brno, Czech Republic, [2]Czech Metrology Institute, Okruzni 31, CZ-63800 Brno, Czech Republic, [3]CEITEC BUT, Purkyňova 123, Brno, CZ–61200, Czech Republic, [4]Institute of Nuclear Physics, Academy of Sciences of the Czech Republic, CZ-25068 Rez near Prague, Czech Republic

09.15-09.30 **The effect of the biopolimers addition on the stability of emulsions of essential oils**
Konrad Terpiłowski[1], Tatiana Demina[2], Michał Chodkowski[1], Elżbieta Grządka[3], Anna Wawryniuk[4], Karolina Czerniejowska[4], Maciej Nastaj[5]
[1]Department of Interfacial Phenomena, Institute of Chemical Sciences, Faculty of Chemistry, Maria Curie Sklodowska University in Lublin, Poland, [2] Laboratory of Solid-State Chemical Reactions, Enikolopov Institute of Synthetic Polymer Materials, Russian Academy of Sciences, Moscow, Russia, [3]Department of Radiochemistry and Environmental Chemistry, Institute of Chemical Sciences, Faculty of Chemistry, Maria Curie-Sklodowska University in Lublin, Poland, [4]Chemical Advisory, Warsaw, Poland, [5]Department of Milk Technology and Hydrocolloids, University of Life Sciences in Lublin, Poland

09.30-09.45 **Processing infrared images as a result of Thermal Non-destructive Testing**
Waldemar Swiderski
Military Institute of Armament Technology, Zielonka, Poland

09.45-10.00 **D-Xylose Dehydration to Furfural in presence of H-Beta Zeolite in water**
Emilija Rakić[1,2], Andrii Kostyniuk[1], Nikola Nikačević[2], Miha Grilc[1], Blaž Likozar[1]
[1]Department of Catalysis and Chemical Reaction Engineering, National, Institute of Chemistry, 19, Hajdrihova, 1001, Ljubljana, Slovenia, [2]Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11000, Belgrade, Serbia

10.00-10.15 **pH-Responsive giant polymeric vesicles prepared via polydimethylsiloxane (PDMS) microfluidics**
Vladimir Sincari, Eliézer Jäger, Jiří Pánek, Martin Hruby and Alessandro Jäger
Institute of Macromolecular Chemistry, Czech Academy of Sciences, Heyrovsky Sq. 2, 16206 Prague, Czech Republic

10.15-10.30 **Electrochemical detection of dihydroxybenzene isomers using carbon supported catalysts**
Kristina Žagar Soderžnik[1], Abhilash Krishnamurthy[1,2]
[1]Jožef Stefan Institute, Jamova cesta 39, 1000 Ljubljana, Slovenia, [2]Jožef Stefan International Postgraduate School, Jamova cesta 39, 1000 Ljubljana, Slovenia

10.30-11.00 **Awards and Closing of the Conference**

11.00 **Cocktail and Greetings for Goodbay to all YUCOMAT participants**

Abstracts

Plenary Lectures

MRS-Serbia 2020 Award

In situ High Resolution Electron Microscopy of Material Reactions, at the Atomic Level

Robert Sinclair and Yunzhi Liu
Department of Materials Science and Engineering, Stanford University, Stanford, CA 94305, USA

This paper gives an overview of how our group has applied in situ observations, under controlled experimental conditions, in a transmission electron microscope (TEM), to understand the mechanism of material reactions, at the atomic scale [1]. Firstly, because of the thin nature of the samples required for high resolution imaging, it must be established that reproducible data can be obtained by this experimental approach. We have provided guidelines to ensure this [2], including, most sensitively, comparison of reaction activation energies determined in situ with those obtained from parallel bulk material. It cannot be emphasized enough how important this is, as in situ observations at the necessary magnifications almost always reveal changes never seen before. The reactions studied include surface and defect re-arrangements in semiconductors, crystallization of amorphous materials, solid-state amorphization reactions in multilayers and at interfaces, metal-mediated crystallization of amorphous carbon, silicon and germanium, and several others (e.g., [1]) Arguably one of the most interesting of all concerns both solid-state amorphization and metal-mediated phase transformation in Cu-Ta multilayers [3], which are purportedly immiscible elements. This turns out to be important for the use of tantalum as a diffusion barrier metal for copper in current transistor technology. Extension to environmental TEM obeservations will also be discussed (e.g., [4]) [1] R. Sinclair, In Situ High-Resolution Transmission Electron Microscopy of Materials Reactions, Mats. Res. Soc. Bull. 38 (2013) 1065-71 [2] R. Sinclair, T. Yamashita, M. A. Parker, K. B. Kim, K. Holloway and A. F. Schwartzman, The Development of In Situ High Resolution Electron Microscopy, Acta Crystallogr. Sec. A 44 (1988) 965-75. [3] H. J. Lee, , K. W. Kwon, C. Ryu, and R. Sinclair. "Thermal Stability of a Cu/Ta Multilayer: an Intriguing Interfacial Reaction." Acta Mater. 47, (1999): 3965-75. [4] A. L. Koh, E. Gidcumb, O. Zhou and R. Sinclair, Observations of Carbon Nanotube Oxidation in an Aberration-Corrected, Environmental Transmission Electron Microscope, ACS Nano 7(3) (2013) 2566-72. [5] The contributions of many group members over many years are deeply appreciated.

MRS-Serbia 2021 Award

MXenes - Two-Dimensional Materials for Future Technologies

Yury Gogotsi
Drexel University, Philadelphia, PA 19104, USA

2D carbides and nitrides, known as MXenes, are among the most recent material families. The field is experiencing very fast growth with the number of papers on MXenes exceeding 1000 per year. Major breakthroughs have been achieved in the past 3-4 years, including the discovery of 2D M5C4 carbides with the twinned layers and CVD synthesis of MoSi2N4, representing a new family of 2D nitrides. Synthesis of dozens of predicted MXenes, demonstration of superconductivity in MXenes with specific surface terminations, stronger interactions with electromagnetic waves compared to metals, metallic conductivity combined with hydrophilicity and redox activity, enable applications in many fields. The scalable synthesis by selective etching allows one to produce substantial amounts of MXenes, opening avenues for largevolume applications. Outstanding mechanical properties of Ti3C2, combined with conductivity and strong interfaces, have been used in polymer, ceramic and metal matrix composites. Reversible redox activity of transition metal atoms in the outer layers of MXene flakes combined with high electronic conductivity led to applications in a variety of batteries and electrochemical capacitors. MXenes are promising candidates for energy storage and related electrochemical applications, but applications in optoelectronics, plasmonics, electromagnetic interference shielding, electrocatalysis, medicine, sensors, or water purification are equally exciting, and several of them are on their way to commercialization.

PL.S.I.1.

The Lithium Battery, from a Dream to a Readiness to Take on Climate Change Materials Opportunities and Challenges

Michael Stanley Whittingham,
Nobel Laureate in Chemistry 2019 for the development of lithium-ion batteries
Binghamton University, State University of New York, US

Lithium-ion batteries have come from an idea in 1972 to dominate electrochemical energy storage today. They are now in a position to enable the large-scale introduction of renewable energy, as well as electrifying transportation, which will leave a cleaner and more sustainable environment for the next generation. There are ample scientific opportunities to further improve their performance and safety. Today’s cells attain only 25% of their theoretical value. However, as the energy density is increased, the safety tends to be compromised. Examples will include: the soft TiS_2 lattice, the layered oxides, $LiMO_2$, and Li_2VOPO_4, a proof of concept for a two-electron transfer. These opportunities and the technical challenges that need to be overcome will be described in order to open up a discussion.

PL.S.I.2.

Bulk nanostructured metallic materials with multifunctional properties: innovative applications and challenges in commercialization

Ruslan Z. Valiev
Ufa State Aviation Technical University, 12 Karl Marx Street, Ufa 450008, Russia Saint Petersburg State University, Universitetskaya nab. 7/9, 199034 Saint Petersburg, Russia

Multiple fundamental and experimental studies in recent years have proved severe plastic deformation (SPD) techniques as a very reliable mechanism to produce nanostructured metals and alloys with significantly improved mechanical and functional properties, the latter affected by several factors, including ultrafine grains and also the atomic structure of boundaries in resulting nanomaterials. This report presents the results of complex studies of the formation of different grain boundaries (low angle and high angle ones, special and random, equilibrium and non-equilibrium with strain-distorted structure as well as with the presence of grain boundary segregations and precipitations) in nanostructured materials processed using SPD with various regimes and routes. This entails the materials with superior multifunctional properties, *i.e.* the combination of high mechanical and functional properties (corrosion and radiation resistance, electrical conductivity, etc.) that are induced by grain boundary design. Particular emphasis is laid on the physical nature and the use of multifunctional nanomaterials in products that are presently or will soon become available for their innovative applications in medicine and engineering as well as some challenges in their commercialization.

PL.S.I.3.

Exploiting structural and compositional instabilities in titanium alloys to optimize properties of components fabricated by additive manufacturing

Hamish Fraser[1], Brian Welk[1], Nevin Taylor[1], Zachary Kloenne[1], Yufeng Zheng[2],
Rajarshi Banerjee[3]
[1]The Ohio State University; [2]University of Nevada-Reno; [3]University of North Texas

This paper begins by reviewing various structural and compositional instabilities in titanium alloys, largely identified by application of analytical aberration-corrected (S)TEM, and their roles in various phase transformations which influence significantly microstructures in processed and heat-treated samples. The specific example of additive manufacturing (AM) of titanium alloys is then addressed. The problem to be solved involves the need to effect an equiaxed microstructure in printed parts, rather than the coarse columnar microstructure that is usually observed. This is done here by the use of dilute alloying, added to increase the probability of solutal undercooling during the rapid solidification experienced in AM. Because these solute additions are above the solubility limit in these alloys, heat-treatment studies were conducted to define the heat-treatment possibilities that avoid formation of intermetallic compounds. The results of these heat treatment studies will be described, and the means of optimizing microstructure in these alloys will be discussed.

PL.S.II.1. - Virtual

Bioinspired Super-wettability System and Beyond Quantum-confined Superfluid: Energy Conversion, Chemical Reaction and Biological Information Transfer

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Biological ionic/molecular channels embedded in plasma membranes play important roles in a wide spectrum of physiological processes such as energy conversion, bioinformation transformation and biochemical reaction etc. On the basis of biological channels, signals can be transmitted from the nerves to brain in the process of vision, smell, audition and tactility. Those crucial functions highly depend on their selective protein-based gatekeepers that allow extremely rapid transit (107 ions per channel in one second). This ultrafast mass transfer stems from the special features of the biological channels, e.g., small size, unique structure and surface charge distribution, which lead to peculiar properties, inducing ultrafast ion and molecule transmission in the form of single strand. From the viewpoint of classical thermodynamics, mass transport across nanometer-scale channel with chemical selectivity should be very slow. In the living system, however, the fast transit of ions and molecules is precisely the state of ultrafast fluid caused by a quantized flow. Biological ion channels show that ultrafast ions and molecules transmission are in a quantum way of single molecular or ionic chain with a certain number of molecules or ions, and we define it as “quantum-confined superfluid” (QSF). The biomimetic systems also exhibit QSF phenomena, such as ultrafast ions transport in artificial ion channels, and ultrahigh water flux in artificial water channels. The introduction of QSF into the fields of energy, chemistry and biology would have significant impact. As a challenge to the traditional theory, the concept of QSF will open up a new field of quantum ionics and promote the development and application of energy conversion materials. The development of QSF reactions will expand the application of nanochannels (even sub nanochannels), promote the development of interfacial catalytic chemistry theory, and open up a new way for the future development of chemistry, chemical engineering and synthetic biology. The introduction of quantum ionics into the field of bioinformatics will provide new technical means for the study of neural signals, overturn the understanding of neural signal transmission in neuroscience and brain science, and expand the development of biophysics, bioinformatics and biomedicine.

PL.S.II.2. - Virtual

Engineering advanced materials through polyphenol-mediated assembly

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The development of rapid and versatile coating strategies for interface and particle engineering is of widespread interest [1]. This presentation will focus on our studies on the formation of a unique class of metal–organic materials, metal–phenolic networks (MPNs). MPNs can be formed on various substrates by simply coordinating polyphenols and metal ions through self-assembly [2,3]. This robust assembly strategy is substrate independent (covering organic, inorganic, and biological substrates) and has been used for the preparation of various materials, including thin films, particles, superstructures and macroscopic assemblies. It will be shown that a range of polyphenols and a library of metal ions are suitable for forming MPNs. The MPN materials are stable at physiological pH but disassemble at acidic pH, thus making them of interest for the intracellular release of therapeutics. By altering the type of metal ions, different functions can be incorporated in the MPN materials, ranging from fluorescence to MRI and catalytic capabilities. Furthermore, synthetic polymer–phenol conjugates have been used as building materials to control the biofouling properties of the MPN materials. Examples of self-healing MPN gel materials [4] and engineered protein-based nanoparticles [5] will also be highlighted. The ease and scalability of the assembly process, combined with the tunable properties of MPNs, provide a new avenue for functional interface engineering and make MPNs potential candidates for biomedical, environmental, and advanced materials applications.

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PL.S.II.3. - Virtual

Intelligent Biomaterials

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The central role of science & technology in advancing healthcare of humans is evident from the ongoing mitigation measures implemented against the COVID19 pandemic, which infected 140 million people and caused three million deaths worldwide. Examples include rapid development of vaccines, range of diagnostic tools for screening of billions of people, facemasks, anti-viral surfaces, and point of care and remote monitoring of patients. Beyond the COVID19 pandemic, the demand for healthcare will accelerate due to stressful modern lifestyles, aging population, new diseases & ailments, unmet clinical needs, and growing demand for better healthcare worldwide. On this backdrop, the R&D investments in healthcare scientific research & innovation are expected to grow in the coming years and decades. Perhaps by 2050, humans will have access to intelligent biomaterials, devices, systems, and methods to perceive own thoughts and redesign own mind! A glimpse of emerging future may be gleaned from the Neuralink (https://www.neuralink.com/), which recently announced a neural interface or in-brain device that could potentially solve neurological challenges from memory loss, hearing loss and vision loss to paralysis, depression, and brain tissue damage. Moreover, with further research & innovation the brain-machine interface will enable humans to access and control external devices via thoughts. This lecture seeks to illustrate the emerging directions of intelligent biomaterials and systems thus enabling future healthcare and well-being. More effective antimicrobial and antiviral surfaces & treatments; tissue engineering & regenerative medicine; neural interfaces & neuro-prosthetics; wearables and personalised healthcare will be deliberated in this lecture.

PL.S.II.4. - Virtual

Engineering human tissues for medical impact

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The classical paradigm of tissue engineering involves the integrated use of human stem cells, biomaterials (providing a structural and logistic template for tissue formation) and bioreactors (providing environmental control, dynamic sequences of molecular and physical signalling, and insights into the structure and function of the forming tissues). This biomimetic approach results in an increasingly successful representation of the environmental milieu of tissue development, regeneration, and disease. Living human tissues are now being tailored to the patient and the condition being treated. A reverse paradigm is emerging in recent years, with the development of the "organs on a chip" platforms for modelling of integrated human physiology, using micro-tissues derived from human iPS cells and functionally connected by vascular perfusion. In all cases, the critical questions relate to our ability to recapitulate the cell niches, using biomaterials, molecular and physical regulatory factors. To illustrate the state of the art in the field and reflect on the current challenges and opportunities, this talk will discuss: (*i*) anatomically correct bone regeneration, (*ii*) bioengineering of the lung, and (*iii*) the use of "organs on a chip" for patient-specific studies of human physiology, injury, healing, and disease.

PL.S.II.5. - Virtual

High Entropy Oxides: Opportunities and Challenges

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High entropy oxides (HEOs) are an emerging class of single-phase solid solutions consisting of multiple cations in near-equiatomic proportion. The field of HEOs has rapidly grown in the last half a decade to include numerous compositions along with several crystallographic structures, e.g., rocksalt, fluorite, perovskites, spinels, pyrochlores, etc. Consequently, the extensive compositional flexibility of HEOs offers the possibility to tailor a plethora of functional properties. Examples of some of their improved functionalities compared to conventional oxides are the enhanced electrochemical cyclic stability, superior ionic conductivity, higher catalytic activity, greater thermal insulation and exotic magnetoelectronic properties. This being the opportunities that can be harvested for future applications, researchers working on HEOs face multiple challenges in terms of precise understanding of their atomistic features, such as local elemental distribution, distortion and bonding characteristics. Hence, the talk will provide an overview of the current state of research on HEOs along with the possible approaches to tackle the aforementioned challenges benefitting future research endeavors.

PL.S.II.6. - Virtual

Stabilization of metastable states for sustainable functionalization -From molecular dispersion to spintronics

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Particulate materials are less stable than a massive single crystal of the same chemical composition, referred as a standard state in the thermodynamics. Functional nanomaterials with crystalline imperfections are thus highly metastable evaluated by excess Gibbs energy [1]. However, many functions of the powdery solids rely upon just such imperfections. Therefore, one of the key issues of materials design is the characterization and control of such imperfections. Imperfection derived function and materials stability is a trade-off issue. Various efforts are paid to control materials stability, *e.g.* via rapid quenching for bulk amorphous state, capping to keep anomalous surface states or intergranular cosegregation. The author tries to demonstrate several strategies for stabilizing such "metastable" functional nanomaterials by his own experimental case studies. Characterization of various imperfections is discussed together with sustainability-conscious preparative processes with controlled metastability. Cases studies include:

- Molecular dispersion of drugs with inert or active excepients [2],
- High antisite disorder of spintronic strontium iron molybdate double perovskites, and
- Nanoglassy states of Li-based pyroxene compounds [3].

Common components of these widespread case studies will be summarized in conjunction with particularities of mechanochemical processes.

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PL.S.II.7. - Virtual

Constitution and Structural Chemistry of T-Mn Systems (T = Sc to Ta)

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Manganese is one of the important alloying partners in many structural alloy systems with Laves-phases as the dominant precipitates. Consequently, the TMn phase diagrams (T is an early transition metal from Sc to Ta) and the TMn2 Laves phases are part of numerous ternary and higher order systems of technological importance, involving hydrogen storage materials, high strength steels (exceeding a yield strength of 700 MPa) and intermetallics in aerospace and/or earth-bound turbine applications and last but not least high strength materials for biomedical applications. Based on our systematic investigations (phase relations, X-ray and neutron structure analyses, SEM, TEM electron diffraction and physical property studies) of binary and ternary Laves phase systems with Mn, the presentation will provide a comprehensive overview on (i) the structural chemistry of the corresponding Mn-based Laves phases, (ii) their thermodynamic stability from calorimetric measurements but also from DFT calculations, (iii) the phase relations in binary T-Mn systems including CALPHAD-type thermodynamic assessments, and (iv) evaluation of physical properties (resistivity, magnetism, specific heat) including also mechanical properties.

PL.S.III.1.

Two-dimensional empty space and its unique properties

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I provide an overview of our recent work on atomic-scale cavities fabricated by van der Waals assembly of 2D crystals. These ultimately narrow structures can be viewed as if an individual atomic plane were extracted from a bulk crystal leaving behind a 2D empty space, essentially an angstrom-size gap connecting two edge dislocations. Gas, liquid, ion and proton transport have been studied using such 2D cavities down to one atom in height, revealing many interesting and sometimes counterintuitive properties.

PL.S.III.2. - Virtual

Advances in molecular beam epitaxy of superconducting materials

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After three decades of innovation and development, atomic-layer-by-layer molecular beam epitaxy (ALL-MBE) has risen to prominence as a paramount technique in Materials science and Condensed matter physics, in particular for synthesis of strongly-correlated-electron materials and superconductors. I will describe three different ALL-MBE systems: one that includes a Time-offlight ion scattering and recoil spectroscopy (TOF-ISARS) system, the second coupled to AngleResolved photoemission spectroscopy (ARPES) and Spectroscopic-Imaging Scanning Tunneling Microscopy (SI-STM), and the third connected to a Low-energy electron microscope (LEEM), Low-energy electron diffraction (LEED) and an in-situ magnetic and transport measurements system. Each of these instruments offers some unique research capabilities, and a representative scientific case will be made for each one. Examples will include delta-doping tomography, synthesis of artificial (metastable) materials, STM and ARPES spectra of materials that do not cleave well in vacuum, and movies of growth of new quantum materials.

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PL.S.III.3.

Nanobiosensors for diagnostics applications

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There is a high demand to develop innovative and cost effective devices with interest for health care beside environment diagnostics, safety and security applications. The development of such devices is strongly related to new materials and technologies being nanomaterials and nanotechnology of special role. We study how new nanomaterials such as nanoparticles, graphene, nano/micromotors can be integrated in simple sensors thanks to their advantageous properties. Beside plastic platforms physical, chemical and mechanical properties of cellulose in both micro and nanofiber-based networks combined with their abundance in nature or easy to prepare and control procedures are making these materials of great interest while looking for cost-efficient and green alternatives for device production technologies. These devices should be ASSURED: affordable, sensitive, specific, user-friendly, rapid and robust, equipment free and deliverable to end-users. How to design simple paper-based biosensor architectures? How to tune their analytical performance upon demand? How one can couple nanomaterials with paper and what is the benefit? Which are the perspectives to link these simple platforms and detection technologies with mobile communication? I will try to give responses to these questions through various interesting applications related to protein, DNA and even contaminants detection all of extreme importance for diagnostics, nanotheranostics, environment control, safety and security.

PL.S.III.4.

The “Chemistree“ of Porous Solids

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That composition and structure profoundly impact the properties of crystalline solids has provided impetus for exponential growth in the field of crystal engineering over the past 25 years. Crystal engineering has evolved from structure design (form) to control over bulk properties (function). Today, especially when coupled with molecular modelling and in situ characterisation, crystal engineering offers a paradigm shift from the more random, high throughput methods that have traditionally been utilised in materials discovery and development. Simply put, custom-design of the right crystalline material for the right application, bespoke materials, is in hand. Porous crystalline materials exemplify this situation. The “node-andlinker“ design concept has afforded more than 100,000 porous coordination networks (PCNs) since it was introduced by Robson and Hoskins in 1990. This has created a challenge for property evaluation since the number of new PCNs being produced exceeds our capacity to evaluate them properly. This is in part because whereas preliminary studies might suggest great promise for separations and/or catalysis, many PCNs are handicapped by cost or performance (*e.g* poor chemical stability, interference from water vapour, low selectivity) limitations. In this contribution, we will present an overview of the “chemistree“ (taxonomy) of porous PCNs and address why their amenability to crystal engineering is critical to enable the creation of platforms of related materials that are ideal for study of structure-function relationships. Two classes of porous materials are of particular interest: Hybrid Ultramicroporous Materials, HUMs, are built from metal or metal cluster “nodes” and combinations of organic and inorganic “linkers”. We have found that the pore chemistry and size (< 0.7 nm) of HUMs can overcome several of the weaknesses of existing classes of porous material. Materials that switch between non-porous (closed) and porous (open) phases can exhibit isotherms that, perhaps counterintuitively, are advantageous in terms of working capacity vs. rigid porous materials. Specific examples of both classes of PCN will be presented and discussed in terms of their performance with respect to important gas separation (*e.g.* CO_2 capture, C_2H_2 capture and natural gas upgrading) and water purification applications.

Oral Presentations

O.S.I.1.

Phase Transformations in a Heterogeneous Ti-xNb-7Zr-0.8O Alloy Prepared by a Field-assisted Sintering Technique

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Ti-xNb-7Zr-0.8O alloy was prepared from elemental powders by a field-assisted sintering technique (FAST). Nb is the main beta-stabilizing element, as well as being the element with the slowest diffusion. A compositional gradient of Nb was produced in the alloy, allowing the observation of phase transformations over a wide range of compositions. Scanning and transmission electron microscopy investigations revealed that Nb-rich regions retained the metastable β phase, surrounded by transition region consisting of the β and ω phases and Nb-lean regions consisting of the α and β phases. The critical concentration of Nb determining whether α or ω will precipitate during cooling was determined to be 22 wt.%. The observed as-sintered microstructure is discussed with respect to the Gibbs free energy curves and the phase diagram. The paper validates the viability of using FAST to prepare heterogeneous alloys permitting the study of phase transformations over a wide range of compositions.

O.S.I.2.

Tuning the thermoelectric performance of $CaMnO_3$-based ceramics by controlled exsolution and micro-structuring

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Oxide-based thermoelectric modules may operate at high temperatures in ambient atmosphere where metal-based devices are ruled out due to thermal instability. Combined with low cost and environmentally benign materials, the oxide-based modules are attractive alternatives in applications such as waste heat harvesting and sensors at high temperatures. Recently it was shown that n-type $CaMnO_{3-\delta}$-based composites ($CaMnO_3/CaMn_2O_4$) demonstrated improved thermoelectric performance compared with pristine $CaMnO_{3-\delta}$ due to enhanced electrical conductivity.

In this work we extend the study on $CaMnO_3/CaMn_2O_4$ composites focusing on the effect of microstructure and composition on the thermoelectric properties. Single phase compositions with rock-salt structure with Mn/Ca ratios larger than unity were produced in reducing atmosphere (5 % H_2 in Ar) and subsequently fully densified by spark plasma sintering in vacuum. Annealing in air at 1340 °C between 1 and 8 hours activated redox exsolution and resulted in a variation in microstructure and materials with 10 and 15 vol% $CaMn_2O_4$, respectively. The nature of the $CaMnO_{3-\delta}$-$CaMn_2O_4$ interface was analysed by scanning electron microscopy (SEM) and transmission electron microscopy (TEM) followed by a theoretical approach based on density functional theory (DFT).

The bulk materials were characterized with respect to electrical conductivity (σ), thermal conductivity (κ) and Seebeck coefficient at temperatures between 300 and 900 °C in air. The highest σ and lowest κ was obtained for composites with 10 vol% $CaMn_2O_4$ (CMO10%8h), reaching 49 $S \cdot cm^{-1}$ at 900 °C and 0.56 $W \cdot m^{-1}K^{-1}$ at 700 °C, respectively. However, the highest zT was observed for samples with 15 vol% $CaMn_2O_4$ (CMO15%8h) reaching 0.11 at 900 °C, due to the enhanced power factor above 700 °C.

O.S.I.3.

Coordination Polymers based on 1,2,4-Triazole

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The five-membered ring system consisting of carbon and three nitrogen heteroatoms (C2N3H3) was named Triazole by Bladin in 1885. This interesting class of heterocyclic compounds and their substituted derivatives to form coordination complexes with transition metals has various applications in the field of medical science, agrochemical research, materials science and pharmaceuticals [1]. Triazole exists as two structural isomers-1,2,3-triazoles and 1,2,4-triazoles. The two tautomeric forms of 1,2,4-triazoles are 1H-1,2,4-triazole and 4H-1,2,4-triazole. Due to the position of the donor atom in the ring, triazoles have the ability to bridge the (transition) metal ions. This bridge offers several different geometries depending on the coordinated metal atom.

The present work deals with the systematic study of the synthesis, structure, electronic and magnetic properties of transition metal [Iron(II), Cobalt(II) and Copper(II)] complexes and coordination polymers with 1,2,4-triazole as a ligand [2, 3]. The iron coordination polymer [Fe(Htrz)2(trz)](BF4) exhibits spin-transition from low spin to high spin state upon heating [4]. It is shown that the crystal size is concentration and temperature dependent. The structure is determined by means of powder X-ray diffraction (PXRD) and single crystal X-ray diffraction (SCXRD) in combination with the vibrational modes studied by Raman spectroscopy. The magnetic properties of the coordination polymer are studied by superconducting quantum Interference device (SQUID) magnetometry. Also, the spectro-electrochemical analysis is carried out to elucidate the redox activity of the complexes and corresponding changes in their optical and electrical transport properties.

Acknowledgements

This work was supported by the Austrian Science Fund (FWF) P30431-N36 and the Czech Science Foundation (GACR) 19-15217S

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O.S.I.4.

Odd-Even Effect in Molecular Packing of Self-Assembled Monolayers of Biphenyl-Substituted Fatty Acid on Ag(111)

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Self-assembled monolayers (SAMs) offer an unique opportunity to change the surface properties of materials using organic molecules in molecular electronics and biosensing devices[1]. Current standard in SAMs formation is based on using sulfur as an anchoring group to the metal substrate. Our analysis indicates that by replacing thiol headgroup by carboxylic[2], a highly interesting alternative for SAMs formation is possible, particularly when 2D ordering, SAM fabrication time and stability in ambient conditions are of great importance. Following this first observation made for a specific system, in the subsequent work we have investigated a homolog series of SAMs based on biphenyl-substituted fatty acids on Ag(111) in the form of $(C_6H_4)_2$-$(CH_2)_n$-COO/Ag (BPnCOO/Ag, n = 1-4)[3]. The series of experiments were carried out using IRRAS, STM and XPS. The results of this combined microscopic and spectroscopic analysis demonstrate very strong dependence of the structural properties on the number of the CH2 groups in the short aliphatic linker. Monolayers with n = even show highly ordered and stable structures. In contrast, SAMs with n = odd have disordered liquid-like structure with more canted orientation of the molecular backbone and the carboxylic headgroup, which results in lower packing density and film thickness compared to the even-numbered SAMs. Our results demonstrate that for BPnCOO/Ag, this odd-even effect is particularly strong and fully controls the ability of molecules to form highly ordered structures. This observation seems to be of key importance for the design of SAMs based on the carboxylic group, which, for correctly designed molecules, forms much better 2D-ordered structures compared to commonly used thiols.

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O.S.I.5.

An in-situ study on phase transformations in metastable β titanium and zirconium alloys

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Titanium and zirconium as elements are in the same group of periodic table and crystallize in the same crystallographic phases. While titanium and its alloys are due to their high specific strength utilized in aircraft industry and due to biocompatiblity in biomedicine, zirconium is used mainly in nuclear reactors as a fuel cladding due to its low cross section for neutron caption.

Metastable β-Ti alloys have unique mechanical and physical properties and are the most studied group of titanium alloys. Their phase transformations have been widely explored. On the other hand, only α-zirconium alloys with low amount of solute elements have been studied and used.

In this study, the knowledge of phase transformations in metastable β-Ti alloys was used to study phase transitions in metastable β-Zr alloys. In-situ methods such as resistivity measurements and synchrotron X-ray studies were applied in order to characterize phase transformations in Zr-(12-18)Nb alloys and, for comparison, in Ti-(12-18)Mo alloys. Despite similar qualitative behaviour quantitative differences were observed and discussed.

O.S.I.6.

Fronts of the Deformation Phase Transformation in TRIP-steel

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The kinetics of the martensitic transformation fronts in chromium-nickel-molybdenum transformation-induced plasticity (TRIP) steel was studied in relation to preliminary thermomechanical treatment using the digital image correlation method. It was found that warm rolling of steel to 40–63% reduction significantly increases the stress of the onset of strain-induced phase transformation and changes the loading curve stages. After austenitization and rolling, the specimens demonstrate an S-shaped loading curve with a pseudo-plateau.The strain-induced phase transformation in TRIP steel occurring through the formation of Lüders and Portevin–Le Chatelier(PLC) bands is shown to be an autowave process of localized plasticity. The austenite → martensite transformation at the elastic-plastic transition occurs in the form of several switching localized plasticity autowaves.

Further plastic flow after annihilation of switching autowaves can occur by martensitic transformation in the form of propagating excitation autowaves, which are mobile PLC band fronts. Regardless of the presence of visible serrations in the stress-strain curve, the PLC band fronts repeatedly pass through the loaded specimen until the strain-induced phase transformation is fully completed.

The interconversion of autowave modes was observed for the first time. It was found that the sources of excitation autowaves in the material are the nucleation or annihilation sites of switching autowaves. The sites divide the material into separate regions in which the straininduced phase transformation processes proceed independently.

Acknowledgments: The reported study was funded by RFBR, project number 20-31-70001

O.S.I.7.

Magneto-optic Janus nanoplatelets

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Janus particles (JP) are attractive type of particles distinguished with different chemical or physical functionalities at their opposite sides. The dual structure of JPs offers an opportunity to exhibit distinct functionalities in a single particle. Among them, magneto-optic JPs present a unique group of materials with many possible applications, such as in vivo cancer imaging, drug delivery, and photothermal therapy. But, preparation of this kind of material is challenging, especially if the core particle is hard-magnetic material with a nanoplatelet shape, as barium-hexaferrite nanoplatelets (NPLs). In the present study, Janus nanoplatelets (J-NPLs) are prepared by employing Pickering emulsion, i.e., Granick's, method, where the emulsion was prepared by mixing two phases wax and water, with addition of NPLs, and surfactant cetyltrimethyl ammonium bromide. Emulsification was done at the temperature higher than the melting point of the wax. During emulsification, NPLs were adsorbed onto wax:water interface. After emulsification, we cooled emulsion to the room temperature, and obtained solidified wax colloidosomes, covered with NPLs. We optimized parameters for the production of colloidosomes: ratio of NPLs surfactant: water:wax, speed of homogenizer, and time of emulsification. Colloidosomes with the best characteristics for the production of Janus NPLs were subsequently treated with mercapto-silane, and gold nanospheres were attached. In the last step, wax was dissolved, Janus NPLs were purified. The formation of the first hard-magnetic Janus NPLs was confirmed by transmission electron microscopy and the effect of applied magnetic field on their optical properties was measured.

O.S.I.8.

Facile Microwave Assisted Synthesis of Silica based nanocoatings with tunable wettability

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Water is one of the most active factor of degradation of many materials, from textile to wood and stone. Thus, liquid repellence becomes an important property for a functionalized solid surface in many industrial as well as biological applications.

The present work reports a simple route for the fabrication of silica nanoparticles based filmogenic materials with suitable combination of chemical characteristics and roughness, in order to produce highly hydrophobic surfaces. The SiO_2 nanoparticles with various size were synthesized by using hydrothermal synthesis using microwave irradiation, as low cost, energy saving approach. The SiO_2 nanoparticles were characterized using dynamic light scattering, transmission and scanning electron microscopy.

The silica based materials were obtained in two step procedure, by functionalizing nanoparticles with various silane derivatives using the sol-gel method, in both normal conditions and microwave irradiation. The as-fabricated nanostructured materials were deposited onto model textile cotton and glass and the wettability of the treated surfaces was evaluated from static and dynamic contact angles using water (surface tension, $\gamma = 72.1$ mN/m) and hexadecane (surface tension, $\gamma = 27.5$ mN/m) as reference liquids. The influence of the organo-silane derivative and size of the pristine SiO_2 nanoparticles on the wettability properties on both glass and textile was investigated. In conclusion, highly hidrophobic to superhydrophobic coatings were successfully prepared, by using a facile two-step microwave synthesis.

Acknowledgements:
This work was supported by grants of the Romanian Ministry of Research and Innovation, CCCDI - UEFISCDI, project number PN-III-P1-1.2-PCCDI-2017-0743/P5, contract 44PCCDI/2018, within PNCDI III.

O.S.I.9.

Oscillation in Stability of Consecutive Chemical Bonds in Self – Assembled Monolayers with Carboxylic Binding Group

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Bonding stability is an essential parameter considering different applications of self-assembled monolayers (SAMs), but probing it is challenging, both experimentally and theoretically. Recently, static secondary ion mass spectrometry (S-SIMS) has been proposed to address this issue [1,2]. Studies on how binding groups and metal substrates alters the stability of the chemical bonds at the molecule-metal interface have been performed using homologous series of SAMs: BP*n*S(Se) (*n*=2-6) on Au(111) and Ag(111). The analysis of S-SIMS data for these SAMs shows positional oscillations in the stability of the consecutive chemical bonds. To prove this approach for other types of molecule-metal interfaces we extended the headgroup from a single atom (S or Se) into a chemical group (COO-), which binds molecules via an ionic bond. To make a direct comparison, we used analogous molecules based on carboxylic acids: BP*n*COO/Ag [3]. By analysing S-SIMS data and performing density functional theory (DFT) calculations, we proved that the effect of oscillation is not limited only to covalent-based interfaces, but is also observed for other types of headgroups [4]. Obtained results revealed that the phase of the respective oscillation for unbounded and bonded to the surface molecule are opposite. Since the phase of measured experimentally oscillations is consistent with the chemisorbed molecules we could, for the first time, directly confirm that emission of investigated fragments takes place directly from the monolayer and is not a result of later fragmentation of molecules desorbed from the monolayer.

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O.S.I.10.

The Odd-Even Effect in Electron Beam Irradiation of Hybrid Aromatic- Aliphatic Self-Assembled Monolayers of Fatty Acid

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Electron irradiation of aromatic self-assembled monolayers (SAMs) in combination with different lithographic approaches provides an interesting alternative for high resolution surface pattering. More recently it has been also demonstrated that this process can be used for carbon nanomembranes (CNMs) fabrication which form technologically attractive 2D materials, with potential application in different areas of nanotechnology such as ultrafiltration and nanobiosensing. To better understand the relation between original SAM structure [1] and resulting CNMs formation [2], in the current study [3] we conduct systematic analysis of the electron irradiation process for a model SAM system deposited on Ag substrates and based on homologue series of biphenyl substituted carboxylic acids (C_6H_5-C_6H_4-$(CH_2)_n$-COO/Ag, n = 2-6) with different length of the aliphatic linker defined by the number n. Our results of X-ray photoelectron spectroscopy of irradiated monolayers show that process of electron induced desorption, cross-linking as well as elimination of the SAM binding group depends on the parity of the parameter n (the *odd-even* effect). Our observations indicate a way for controlling thickness and purity of such nanomembranes, which are the key parameters determining the range of CNMs applications.

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O.S.I.11.

Super porous hydrogels based on poly(N-isopropylacrylamide) for potential application as soft actuators with extreme-fast volume responsive temperature- and pH-sensitive properties

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The macroporous nanocomposite hydrogels based on poly(N-isopropylacrylamide)/nano-SiO_2 were successfully prepared and investigated. The incorporation of nano-SiO_2 as a filler (formed in-situ via hydrolysis/condensation of tetramethoxysilane during the cryo-polymerization) seems to strongly raise the modulus and also reinforces the pore walls against collapse during deswelling. The gels are able of ultra-fast deswelling and re-swelling (5.5 s for 70 % in both directions) in response to *T* and additionally introducing pH-responsiveness into the gels was the main goal of this work. It was managed by using another co-monomer - sodium methacrylate (1–10 mol% of SMA) to the synthesis. A noticeable pH-responsiveness was achieved for 1 mol% of SMA, while for the best dual responsiveness (to T and pH) SMA-contents, 3–5 mol% were found to be optimal. On the other hand, increasing SMA content highly reduces the T-responsiveness of the prepared hydrogels. The rate of pH-response was found to be much slower than in case of the *T*-response: 75 s were needed for 70 % of de-swelling, and 90 min for 70 % of re-swelling. This behaviour could be explained by different mechanisms of stimulus propagation (momentum transfer for *T*, vs. diffusion for pH) and by the mechanical effect of a contracting stiff and porous surface layer (much faster pH-deswelling than re-swelling). Due to the above-mentioned properties, super porous hydrogels could be act as soft actuators with extreme-fast volume response to temperature and slower response to pH.

Acknowledgements: The authors thank the Czech Science Foundation, project Nr. 19-04925S for financial support of this work.

O.S.I.12.

Electrochemical Reduction of CO_2 on Electrodeposited Copper-based Nanoparticles: Identical Location Electron Microscopy Stability Study

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Rapid industrialization and modernization of today's society have led to anthropogenic emissions that inevitably affect climate change. Up to date, an enormous increase of atmospheric CO_2 (~ 400 ppm) has triggered various solutions and efforts to decrease emission, likewise to deal with Paris Agreement to limit the global warming below 2 °C, compared to pre-industrial level. Electrochemical reduction of CO_2 (ERC) comes to the fore as one of the perspective ways to convert CO_2 to chemical fuels and other energy-dense products, powered by renewable energy. Copper is the only monometallic catalyst that can produce hydrocarbons and alcohols in decent amounts.[1] However, severe changes to its morphology and structure are observed upon exposure to the ERC operation conditions. To bring the ERC process to an industrially relevant level, the stability of copper-based catalysts must also be evaluated.[2] Among the various techniques of synthesis of copper-based catalysts for ERC, electrodeposition stood out as a generally inexpensive, simple and versatile method for obtaining copper nanostructured materials. The stability of pulse-electrodeposited copper nanoparticles under relevant ERC conditions tracked with identical location scanning electron microscopy (IL-SEM) method will be discussed. This approach provides direct evidence of the history of the tracked changes to the observed Cu nanoparticles. With this objective information, we could explain the observed structural changes with two separate electrochemical processes occurring one after another, namely copper dissolution copper and subsequent redeposition of the dissolved copper species in a form of new smaller Cu fragments.[3]

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O.S.I.13.

Catalyst Screening for Homogeneous and Heterogeneous Carboxylation of Lignin-derived Model Compounds

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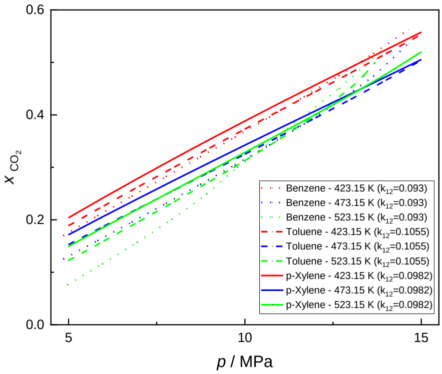
The narrow list of possible substitutions for fossil resources suggests lignocellulose and carbon dioxide as the two that are abundant, easily replenished, and offer various opportunities for further upgrading. Lignin is an aromatic polymer obtained from depolymerization of lignocellulose, which can further yield variety of model compounds through wide assortment of chemical treatments. Carboxylation is one of the possible routes, which therefore finds the use for poorly utilized lignin, as well as widely available and environmentally harmful carbon dioxide. The literature offers various reaction routes and conditions using homogeneous catalysis, complex, toxic additives, and demanding separation methods. Therefore, the search for simple, non-toxic, and reusable catalysts for carboxylation reactions under moderate reaction conditions is ever growing. The reaction conditions governing the activity of selected catalysts is of utmost importance regardless of their nature.



Dissolution of CO_2 in the solvent used for carboxylation process has significant role in the reaction efficiency. The solubility of CO_2 in benzene, toluene and p-xylene was correlated in this work at temperatures (423.15-523.15) K and pressures (5-15) MPa by using Soave-Redlich-Kwong (SRK) equation of state. It was noticed that solubility of CO_2 in all studied solvents decreases with increase in temperature and rises when pressure goes up. The differences in the amount of dissolved CO_2 are higher at lower temperatures, while at temperatures above 423.15 K they are not so significant. Further, the addition of methyl group to benzene ring increases the solubility of CO_2, *i.e.* among the studied solvents CO_2 dissolves best in p-xylene and worst in benzene. The results presented at the conference will show an influence of various reaction conditions on solubility of CO_2 in the selected solvent, and the activity and selectivity of X-Cl and silver-based catalysts for carboxylation of various lignin-derived model compounds.

Acknowledgments: Authors gratefully acknowledge financial support by the Slovenian Research Agency (P2-0152 and J2-1723).

O.S.I.14.

Novel Magnesium Alloy Mg-4Gd-4Y-2Ca with enhanced ignition temperature and mechanical properties

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Novel magnesium alloy Mg-4Gd-4Y-2Ca (wt.%) is designed as a light-weight material for manufacturing aircraft parts. The alloy is characterized by good mechanical properties and exceptionally high ignition temperature, which is a critical safety measure. The material was prepared by casting and subsequently processed by extrusion at temperatures of 350 and 400 °C. The effect of extrusion on the microstructure, mechanical properties and ignition temperature is studied. The obtained results indicated a substantial effect of the extrusion temperature on the average grain size, the recrystallized fraction and texture formation. Microstructure condition directly affected the tensile and compressive behaviour with an observed average tensile yield strength of 302 MPa and 272 MPa for materials extruded at 350 and 400 °C, respectively. Both conditions featured a high ignition temperature of ≈1100 °C, which was attributed to the synergic effect of Y, Gd and Ca oxides, with the dominant effect of Y_2O_3. The achieved combination of enhanced mechanical properties and the ignition temperature makes this novel alloy a prominent candidate for more ecological aircraft applications.

O.S.I.15.

Properties of belite-calcium sulfoaluminate cements synthesized from various industrial residues

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This study focused on the preparation of low carbon belite-calcium sulfoaluminate cements (BCSA), where certain amounts of raw materials were replaced with different secondary raw materials. By adding industrial residues to the raw mixture, bauxite - a limited and often expensive source of aluminium - was also replaced, either partially or fully. Cement clinkers with a targeted phase composition of 65 wt. % belite (C_2S), 20 wt. % calcium sulfoaluminate ($C_4A_3\acute{S}$) and 10 wt. % ferrite (C_4AF) were synthesized. Industrial mineral residues from thermal power plants, the paper industry, steel plants, and mining activities were considered for the study. It was possible to incorporate between 10.1 and 57.7 wt. % of secondary raw material, depending upon its chemical composition. Furthermore, cements with a calcium sulfate to calcium sulfoaluminate ratio of 1.5 were prepared. To eliminate the effect of particle size on reactivity all cements were ground to a similar Blaine specific surface area. The results showed that, besides the main clinker phases, minor phases such as periclase, mayenite, and gehlenite also formed. In order to evaluate the influence of incorporating various industrial residues on the composition of cement clinkers, and consequently the properties of the cement, reactivity and heat evolution were studied by isothermal calorimetry. Furthermore, the evolution of compressive strength was investigated, and the phase composition during hydration was studied by X-ray powder diffraction as well as quantitatively using the Rietveld method. Differential thermal analysis and thermogravimetric analysis were also carried out in order to support and complement the identification of hydration products through X-ray powder diffraction. Differences in compressive strength, reactivity and the phase assemblages of cements were observed depending on the type of secondary materials used in the cement clinkers.

Acknowledgment: The study has received funding from the European Institute of Innovation and Technology (EIT), a body of the European Union, under Horizon 2020, the EU Framework Program for Research and Innovation (RIS-ALiCE , project no. 18258).

O.S.I.16.

Microkinetic Study of Furfural Hydrotreatment over Various MoO$_x$-Based Catalysts

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As the world is facing problems associated with increasing energy usage, their limited supply, and further environmental concerns related to their consumption, the demand for renewable fuels is therefore increasing as well. Furfural is a platform chemical obtained from lignocellulosic biomass, which can be further upgraded to a variety of compounds that find their usage as fuel additives and value-added chemicals. Catalytic hydrotreatment of furfural in isopropanol, over bulk MoO$_x$ catalysts has been shown to successfully convert furfural to isopropyl levulinate, under mild conditions. A systematic study has been carried out in order to obtain mechanistic and kinetic insight into furfural hydrotreatment. Three MoO$_3$ catalysts obtained from various manufacturers, MoO$_2$, Mo$_2$C, MoO$_3$-NiO/Al$_3$O$_2$, and WO$_3$ (shown in Fig. 1) have been primarily used to compare their activity. After obtaining most active catalysts (MoO$_2$ and MoO$_3$-F), further testing was carried out to observe effects of reaction conditions: temperature, pressure, catalyst loading, and starting reactant concentration. GC-MS analyses using Shimadzu 2010 Ultra have been used to propose a detailed reaction pathway, which was further utilized in microkinetic modelling. The obtained kinetic data agree relatively well with the extensive experimental results. Results presented at the conference will show an influence of wide array of reaction conditions on the activity and selectivity of various MoO$_x$ catalysts for the hydrotreatment of furfural.

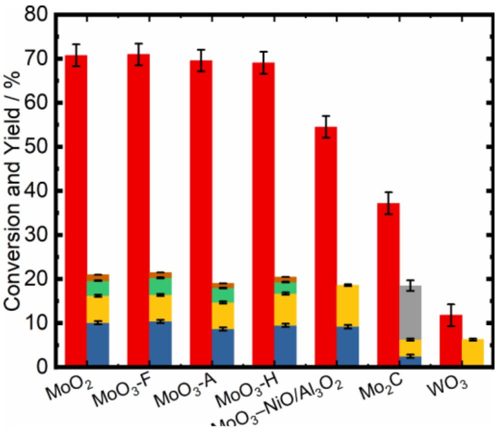

Fig. 1. Catalyst screening results obtained after 1.5 h at each temperature step of 125, 175, and 225 °C. Results shown represent conversion of 10 wt.-% 🟥 FUR, and yields of 🟦 IPL, 🟨 IFE, 🟩 FAC, ⬜ FAL, and 🟧 ALAC, at the end of the reaction.

Acknowledgments: Authors gratefully acknowledge financial support by the Horizon 2020 Program under Grant agreement no. 814416 (ReaxPro) and ARRS (P2-0152 and Z2-9200).

O.S.I.17.

Microstructure and corrosion properties of a novel biomedical WN43 magnesium alloy prepared by spark plasma sintering

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A novel magnesium-based WN43 (Y - 4 wt%, Nd - 3 wt%) alloy was prepared by the method of powder metallurgy. A modern spark plasma sintering technique was used to effectively produced WN43 samples from gas-atomized powder. Different sintering temperatures from 400 °C to 550 °C and two holding times of 3 and 10 minutes were used. The effect of the sintering parameters, particularly sintering temperature and holding time, on microstructure and corrosion properties was investigated. High dense material was obtained in all investigated specimens. The microstructure of powders and compacted samples were observed by scanning and transition electron microscopy. Increasing the sintering temperature and prolonging the holding time results in uniform recrystallization and grain growth accompanied by dissolution and precipitation of new secondary phases. Corrosion properties of compacted samples were evaluated by immersion and by electrochemical tests using NaCl solution. Due to microstructural changes, we obtained an improvement of corrosion characteristics. Moreover, it was shown that a great variety of corrosion characteristics can be obtained by altering the SPS parameters so as to fulfil case-specific requirements typical of biomedical materials. Consequently, the novel WN43 alloy prepared by SPS seems to be a particularly suitable material for biomedical use.

O.S.II.1.

Are high-entropy alloys better than conventional ones?

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In spite of a huge expansion of the research on high-entropy alloys (HEA) their basic understanding is still limited, which is detrimental both for the design of HEAs and for their application. Nevertheless, some properties of a few HEA exceed those of conventional alloys (CA). Clearly, the study of transition from HEA to CA composed from the same constituents is very important both, for understanding the formation of HEA and for proper evaluation of their potential in respect to that of CA. However, this transition has so far been studied in only two types of alloys: crystalline CrMnFeCoNi alloys [1] and amorphous TiZrNbCuNi/Co alloys [2]. Here we review the effects of the transition from HEA to CA on selected properties of these alloys. In both systems the variation of a given property with composition depends sharply on the selected principal component (thus on the interatomic correlations and related electronic structure) and can be either monotonic, or nonmonotonic.

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O.S.II.2.

Photocatalytic and Photoelectrocatalytic Degradation of Organic Compoundsin TiO_2-nanotubes-based Reactors

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Anodic oxidation of Ti metal is a method of choice for synthesis of highly ordered polycrystalline TiO_2 nanotubes that are firmly attached to the titanium metal substrate. Easy control of TiO_2 nanotubes' length, possibility to modify TiO_2nanotubes'chemical composition and the possibility to tailor TiO_2 nanotubes with metallic nanoparticels, make suchTiO_2/Ti substrate heterostructures applicable for photocatalytic as well as for photoelectrocatalytic degradation of organic compounds in waste waters. Furthermore, strong adhesion of ingrown TiO_2 nanotubes into the titanium substrate prevents possible release of TiO_2 particles into liquid after the purification process is complete thus preventing subsequent pollution of purified liquid. In our work we have systematically studied the influence of various experimental parameters of anodic oxidation process (surface preparation of metal titanium, electrolyte aging, applied potential, time of anodization, thermal treatment, etc.) on TiO_2 nanotubes structure and morphology (length, crystallinity, crystal structure, inner and outer diameter of TiO_2 nanotubes, etc.). Microstructural examination of these nanostructures showed that TiO_2nanotubes are polycrystalline in nature with nano-grains up to app. 10 nm, exhibiting anatase crystal structure. The inner and outer diameter of the nanotubes ranged from 50 to 60 nm and from 100 to120 nm, respectively. Thus, prepared TiO_2 nanotubes arrays were incorporated into specially designed photocatalytic and photoelectrocatalytic (micro)reactors. In order to study efficiency of these catalytic systems, degradation studies of caffeine, phenol and synthetic dye were performed. Kinetic studies and mechanisms of degradation were also obtained for these compounds. It was found out that partial or complete degradation of chosen organic compounds was achieved in relative short time even at higher flow rates. Even after prolonged degradation tests the TiO_2 nanotubes showed only minor changes in surface morphology and catalytic activity.

O.S.II.3.

Self-organization of plasma in DC and RF magnetron sputtering

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In recent years, imaging studies performed by high-speed cameras and other analytical techniques have demonstrated that magnetron plasma is localized in dense regions called spokes or ionization zones [1,2]. These plasma structures self-organize in periodic or quasi-periodic patterns, exhibit triangular shape, and rotate with velocities of several km/s. The presence of spokes in magnetron plasmas is universally observed in all types of magnetron regimes. In this talk, we will discuss plasma self-organization in DC magnetron sputtering (DCMS) and RF magnetron sputtering (RFMS) regimes [3].

The magnetron plasma was studied by an intensified CCD camera and electrical probes. We explored plasma self-organization for a range of working gas pressures and discharge currents. The number of spokes in the RFMS was always larger than in the DCMS when the discharge was operated at the same pressure and discharge power. The number of spokes increased with the increasing gas pressure for both regimes. The influence of discharge power on the number of spokes was less pronounced. These observations imply that the plasma self-organization is related to the electron energy dissipation, which occurs due to collisions with the atoms of the background gas. To validate this hypothesis, we examined inelastic collisions between electrons and argon atoms. We calculated the dissipation of electron energy in the drift direction and compared the calculations to the length and number of spokes for specific discharge conditions. Overall, the calculations agree well with the observed lengths and number of spokes for both regimes.

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[2] M. Panjan *et al. Plasma Sources Sci. Technol.*, **24** (2015) 065010
[3] M. Panjan *J. Appl. Phys.* **125** (2019) 203303

O.S.II.4.

PLD growth of functional oxides on graphene oxide-buffered silicon surface

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Epitaxial integration of complex oxides with semiconductors is alleviated by the weak van der Waals interactions when the 2D materials are used as buffer layer. As a result, graphene can allow remote epitaxial registry with a substrate at a long distances or act as a template by itself. In the present work, we demonstrate integration of functional oxides ($SrTiO_3$ (STO), $Pb[Zr_{0.52}Ti_{0.48}]O_3$ (PZT) and $LaMnO_3$ (LMO)/STO superlattices (SLs)) with silicon surface that was buffered by a layer of spin-coated graphene oxide. The results reveal that GO can direct the growth of STO to a smooth, compact and pinhole-free layer, with mostly (001) out-of-plane orientation. When this was combined with SrO-assisted deoxidation of silicon surface, a partially epitaxial, highly crystalline STO film, with exclusively (001) out-of-plane orientation, was obtained. As-obtained STO was successfully used as a pseudo-substrate for integration of PZT, that exerted properties comparable to ones obtained in more complex integration methods. Also, very good results were obtained in the case of LMO/STO SLs, with the properties comparable to SLs grown on other buffer layers including: a single-layer buffer of STO prepared by molecular beam epitaxy (MBE) and pulsed laser deposition (PLD), a multilayer buffer of Y-stabilized zirconia/CeO_2/$LaNiO_3$/STO and STO-coated two-dimensional nanosheets of $Ca_2Nb_3O_{10}$ (CNO). Our results suggest that GO can be used a template for integration of complex oxides with silicon in a way that is less demanding in terms on interface control and vacuum conditions, which are important advantages for development of large area PLD processes.

O.S.II.5.

Deposition of metal hydride films by hydrogen transport via a hollow cathode discharge

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The fabrication of thin films of polycrystalline silicon using a reversible chemical reaction was described about 30 years ago by the group of Stan Vepřek of the University of Zurich. They reported that pieces of silicon exposed to a low-pressure high-density hydrogen plasma promoted the formation of volatile silicon hydride, this could then be transported within the reactor to a hot substrate where the decomposition of the hydride resulted in the deposition of silicon thin films. Similarly, hydrogen plasmas have also been used for chemical etching of various materials and, for example, in the case of the deposition of diamond films the preferential etching of sp2 bonded carbon is considered to be of fundamental importance for the formation of diamond-like carbon. In this paper we describe the chemical etching of molybdenum and tantalum by atomic hydrogen generated in a RF or pulsed DC plasma-activated in a hollow cathode. The water- cooled cylindrical cathode was lined with the appropriate metal.

The metal hydride vapour generates in the plasma flowed to quartz substrates which were maintained at temperatures greater than 300 ^{o}C. Under these conditions the metal hydride was thermal decomposed, and a thin film was deposited. A special substrate heater was constructed such that the four quartz substrates used could be simultaneously exposed to the metal hydride vapour, but with each substrate at a different temperature: each approximately 20 ^{o}C less than the neighbouring one. In this way, depositions under identical conditions could be carried out, but at four different temperatures. We report the deposition rate as a function of the substrate temperature and the plasma power and type applied to the hollow cathode, as well as some of the characteristics of the deposited films.

O.S.II.6.

Combustion synthesis of multilayer Ti–Ta–Ni–Ceramic Composite

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Design of materials that combine properties of ceramics and metals, such as hardness, strength, heat resistance, high-temperature strength, wear resistance, and ductility is a popular trend in materials research and design. As is known, combustion-assisted processes can be applied to joining such dissimilar materials. This work aims at the combustion synthesis of layered composite materials from the Ti–Ta–(Ti+0.65C)–Ni–(Ti+1.7B)–(Ti+1.7B)–Ta–Ni–Ti foils and the study on concomitant rapid high-temperature reactions in these systems. The new approach in this work is to pre-alternate layers of refractory metallic foils and reactive tapes to obtain multilayer composite materials. The reactive ceramic-forming (Ti+0.65C) and (Ti+1.7B) tapes were prepared by rolling of a powder blend. Then, the samples comprised of metal foils and reactive ceramic-generating tapes were ignited in a combustion chamber under Ar. The combustion process was monitored with a rapid camcorder and set of thermocouples. Combustion products were characterized by SEM, EDS, XRD, and mechanical testing.

Thin plates of multilayer Ti–Ta-ceramic composite of reduced density have been prepared by combustion-assisted joining between dissimilar materials. Based on SEM results we didn’t observe any visible boundaries between the foils and reactive tapes in the multilayer composite material. Our obtained results can be recommended to fabricate new refractory composite materials with the required structure and properties.

This work was financially supported by the Russian Foundation for Basic Research (project no. 20-08-00594-a).

O.S.II.7.

Reversible intercalation/deintercalation of lithium ions within γ-LiV_2O_5 polymorph

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The electrochemical insertion of lithium ions in V_2O_5 produces various crystal structures depending on lithium concentration. Compositions with lithium content in the range of $1 \leq x \leq 1.8$ take orthorhombic γ-$Li_xV_2O_5$ form. γ-$Li_xV_2O_5$ is capable to accommodate more than one lithium ion per formula unit and therefore interesting to be used as a cathode of lithium-ion battery. Here are presented electrochemical performances of γ-LiV_2O_5 obtained through solid-state reaction. Before galvanostatic cycling the as-synthesized powder is characterized by X-ray powder diffraction, field emission scanning electron microscopy, and FTIR spectroscopy. The crystal structure of the powder is refined in the orthorhombic Pbnm space group. During galvanostatic cycling in a large potential window capacity decrease is observed. In order to reveal the origin of capacity decay the bond valence analysis was performed. It provided a model of lithium diffusion network for the γ-$Li_xV_2O_5$ phase, as well as for the end members obtained at low and high voltages.

O.S.II.8.

TRIP/TWIP effect in beta Ti alloys with high oxygen content

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TRIP/TWIP effect causing high ductility due to martensitic transformation (TRIP) or twinning (TWIP) during loading was observed in beta Ti alloys. Typically, such alloys exhibit high ductility and very pronounced deformation strengthening, but their yield point is low. Controlled concentration of oxygen causes interstitial strengthening. The aim of the research was to develop an alloy with enhanced strength and TRIP/TWIP effect.

Various Ti-Nb-Zr-O based compositions have been prepared by compaction and homogenization via field assisted sintering technique (FAST). Individual compositions have been studied by scanning electron microscopy and microhardness mapping. Compression tests were performed with simultaneous in-situ measurement of acoustic emission and digital image correlation (DIC). The deformed microstructures were analysed by electron back-scatter diffraction (EBSD). Stress induced martensite and {332}<113> twinning was found in a sample with 0.5 wt.% of oxygen and 7 wt.% of Zr.

O.S.II.9.

Non-oxidative dehydrogenation of propane on chromium(III) oxide: an ab initio study of reaction kinetics and catalyst deactivation

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Propylene is traditionally produced in petroleum refineries with steam cracking and fluid catalytic cracking. As these processes cannot keep up with the increased demand for propylene, new sources are being utilized, necessitating new processes. Dehydrogenation of propane, which is a constituent part of natural gas and a by-product of petroleum refining, is a viable alternative. Industrially the most commonly used is the CATOFIN® process, where alumina-supported chromium oxide catalysts are used at 850 K and 1.2-1.5 bar. Propylene and hydrogen are produced in the non-oxidative dehydrogenation process.

In this work, we study the mechanism of propane dehydrogenation on Cr_2O_3(0001) using DFT+U calculations and kinetic Monte Carlo simulations. The catalyst is modelled as a 12-layer chromium-terminated slab. All possible elementary reactions were included, yielding propylene, propyne, and hydrogen. Coking and catalyst deactivation was explicitly taken into account. The kinetic simulations were performed on a 20×20 lattice with two types of active sits (800 in total).

Under the relevant reaction conditions (1 bar propane, 850 K), propylene is the main product. The reaction has an apparent activation barrier of 1.37 eV and order of 1.05. The reaction mostly follows the pathway: $C_3H_8 \rightarrow CH_3CHCH_3 \rightarrow CH_3CHCH_2 \rightarrow CH_3CCH_2 \rightarrow CH_3CCH$. The formation of propyne and cracked products (methane, ethane, ethylene) is negligible but quickly increases at higher temperatures. The dominant cracking reaction is $CH_3CH_2CH_2 \rightarrow CH_3CH_2 + CH_2$. The deactivation of the catalyst is due to the formation of CH_3CC and C* species, which saturate the active sites. Their formation can be described with kinetic parameters of $A = 1.7 \cdot 10^{10}$ s^{-1} and $E_A = 2.82$ eV. At 950 K and 5 bar propane, the catalyst loses half of its active sites after 46 days.

The results are consistent with existing experimental endeavours and microkinetic descriptions. They provide detail insight into the reaction mechanism and allow for fine-tuning of catalysts in the future.

O.S.II.10.

Correlation between the evolution of precipitates and microhardness in Inconel 625 fabricated by laser powder bed fusion

Transferred to Virtual Offline Pesentations

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The aim of this study was examination of the evolution of precipitates and microhardness in the Inconel 625 additively manufactured by laser powder-bed fusion (L-PBF) and subsequently annealed for 5, 100 and 500 hours at 600, 700 and 800 °C. Microstructural investigation was performed by light microscopy, scanning and transmission electron microscopy combined with microanalysis of the chemical composition by energy-dispersive X-ray spectroscopy. Size distribution and volume fraction of the precipitates were determined by means of image analysis. Microhardness measurements were performed with the Vickers indenter at the load of 9.807 N (HV1).

The microstructure of L-PBF Inconel 625 after stress-relief annealing consisted of melt pools with fine grains and cellular-dendritic substructure, where precipitates are located in the cell walls. As a result of annealing at a temperature of 600 °C up to 500 h and at 700 °C for 5 h, the breaking of the cell walls and precipitation of the γ'' phase occurred. The prolongation of annealing at 700 °C up to 100 and 500 h led to the precipitation and subsequent growth of the δ phase, Laves phase, and $M_{23}C_6$ carbides. An increase of temperature up to 800 °C led to significant growth of precipitates. The observed evolution of the microstructure was correlated with the changes in the microhardness. For specimens annealed at 600 °C the highest microhardness of 379 HV1 was obtained after 100 h, while at 700 °C and 5 h it reached 397 HV1. It was concluded that the hardening was caused by the precipitation of the finely dispersed particles of the γ'' phase, coherent with the γ matrix. The prolongation of the annealing at 600 and 700 °C or increase of the temperature to 800 °C resulted in lower hardness. After annealing at 800 °C for 500 h, it was equal to 421 HV1. The drop in microhardness was related to the over-aging, mainly by the coarsening of the δ, Laves and $M_{23}C_6$ precipitates.

The results have shown that the stress-relief annealing of the L-PBF Inconel 625 followed by the short-term annealing at 700 °C for 5 h can lead to the pronounced precipitation hardening by the coherent γ'' phase.

O.S.II.11.

Thin and Thermally Stable SAMs for Formation of Higly Conductive or Higly Insulating Organic Monolayers on Metals

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Self-assembled monolayers (SAMs) on metal substrates are an important part of modern interfacial physical chemistry and advanced nanotechnology. The robustness of SAMs strongly depends on their thermal stability, which, together with electric conductivity, are the key parameters for their applications in molecular/organic electronics and photovoltaics. In this context, using a multidisciplinary approach, we address here the structure, thermal stability and conductivity of SAMs formed on metal substrates (Au or Ag) using different bonding groups such as thiols, selenols, carboxylic acid and carbenes. Our recent results indicate possibility of formation thin well, defined monolayers which exhibit exceptionally high thermal stability and are either highly insulating [1] or highly conductive [2] which makes them an interesting nanomaterial for modification of gate or drain/source electrodes in OFET devices, respectively.

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O.S.II.12.

Porous monolithic 3D nanostructures and nanocomposites based on alumina hydroxides

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The synthesis methods of nanomaterials mostly provide them in the form of dispersed systems. However, high surface energy and topochemical reactions in dispersed systems lead to agglomeration of nanoparticles and clusters, which significantly affects their physicochemical properties and limits their applications. We see the solution of this problem in the development of new synthesis methods that make it possible to obtain nanomaterials with stable physicochemical and structural properties. One of these areas are the porous materials and nanostructures, in which 1D or 2D nanoparticles form stable contact interfaces and combined into a 3D network.

Our research were focused on the study of the following processes: 1. Low-temperature oxidation (T <300 ° C) in a humid gas environment of the surface of binary liquid metal solutions Me (Al), where Me = Hg, Ga, In, Bi, Sn, Pb; 2. The mechanism of formation and growth of highly porous monolithic 3D nanostructures consisting of aluminium oxyhydroxides (PMAO) at the liquid metal surface; 3. Evolution of the chemical composition, structure and morphology of the basic elements of the 3D structure – the nanofibrils during annealing in the temperature range 25 - 1700 °C. During high-temperature annealing monolithic 3D structure of PMAO is preserved, while the samples dimensions decreasing isotropically. The range of the density changes from ~0.02 to ~3 g / cm^3, the porosity decreases from 99 to 25 % and the specific surface decreases more than 100 times. We proposed a simple physical model, describing quantitatively the evolution of the 3D structure and nanofibril's morphology in the temperature range 25 - 1700 °C.

Annealing of PMOA provides additional opportunities for the development of new technologies for practical use. Nanocomposites based on PMAO are a universal basis for the creating functional nanomaterials with a wide range of potential applications: nonlinear optics (photonic crystals, optical elements IR, THz, and GHz), sensor devices. There is a successful experience of using PMAO nanocomposites in photocatalysis: purification of water and air from organic pollution, photodestruction of microorganisms and bacteria.

O.S.II.13.

Ordered structures formation in multicomponent polysaccharide systems; effect of graphene oxide

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Numerous studies indicate fair ability of water soluble polysaccharides including their blends and nanocomposites to form organized structures in solutions and gels. E. g., fibrillar structure and network formation was found in aqueous solutions and gels of methylcellulose (MC) while even thermo-reversible fibrillation of MC/cellulose nanocrystal-based hydrogels was found. Surprisingly, formation of these structures in rigid polysaccharides (mostly films) and their impact on mechanical performance were reported less frequently. The presented study deals with an unknown unexpected effect of 2-hydroxyethylcellulose (HEC) on structure and mechanical performance of methylcellulose (MC) films. This leads to synergistic as well as antagonistic effects on mechanical performance in dependence on modifiers content and ratio. The values of modulus of MC containing 5 and 10 % HEC exceed those of the linear model, which indicates synergistic effect consisting in formation of ordered structures. At the same time, higher content of HEC leads to worse properties indicating dominant contribution of its lower parameters. In spite of absence of direct insight into the structure, combination of XRD, polarized light microscopy and rheology indicates a high effect of small content of HEC on formation of favorable ordered structures and a slight hindering effect of GO on this process. Rheological evaluation indicates ability of HEC to support formation of ordered structures in MC also in water-solution. Important result is that unlike high reinforcing effect of low graphene oxide (GO) content on single MC and HEC components, its presence in blends decreases mechanical properties as a result of disturbing of HEC-induced structural transformations. Further unexpected feature is that negative effects of higher HEC content on mechanical performance are enlarged by GO. The results confirm complex effect of blending and GO on structure and properties of the MC/HEC system.

This work was supported by Czech Science Foundation (Grant No 19-06065S)

O.S.II.14.

ZnO nanoparticles with optimized surface-to-bulk defect ratio for potential biomedical application

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Due to tunable opto-electronic properties ZnO-based nanoparticles (ZnONPs) have been used for application in electronics, optoelectronics, photo(electro)catalysis, etc. Besides, as bio-inert, ZnONPs have a great potential in medicine for biosensing, bioimaging, drug and gene delivery, implants or as antimicrobial and anticancer agents. One of suggested governing mechanism of the biological activities of ZnONPs is based on the formation of reactive oxygen species (ROS). Actually, when ZnONP absorb photon with energy equal or greater than its band gap, electrons (e^-) are excited from the valence band (VB) to the conduction band (CB) leaving the holes (h^+) in VB. In following, the photogenerated h^+ and e^- migrate from bulk to surface. The photogenerated h^+ at the VB react with water molecules adsorbed at the particle surface to produce hydroxyl radicals ($OH^\bullet$), while e^- in CB react with oxygen molecules generating anionic superoxide radicals ($O_2^{-\bullet}$). Radicals can be transformed in highly reactive hydroxyl radicals and so on. Derivatives of this active oxygen can damage the bacterial/tumor cells. However, in sufficiency ROS can damage normal cells as well. Thus, an understanding of ZnONPs crystal structure-activity relationship is crucial for the design of materials safe for application in treating diseases like cancer.

In this study we established correlation between the surface-to-bulk defects ratio in ZnONPs and ROS formation. To vary surface-to-bulk defects ratio, series of ZnONP samples were synthesized by microwave processing of precipitate in the presence of a different amount (5, 10 and 20 wt.%) of surfactants, precisely, CTAB and citric acid. The particles crystallinity and phase purity were investigated by X-ray diffraction, Raman and FTIR spectroscopy. The particles morphology and texture properties were observed with FE–SEM and BET, respectively. The optical properties were studied using UV–Vis DRS and PL spectroscopy. ZnONP samples with different surface-to-bulk defect ratio were examined on ROS formation. Surface-to-bulk defect ratio in ZnONP was correlated with ROS formation, besides; their influence on cytotoxicity to normal and cancerous cells was comprehended.

O.S.II.15.

Identical Location Transmission Electron Microscopy Coupled With Modified Floating Electrode Characterisation of Pt-Co/C Electrocatalyst for Oxygen Reduction Reaction

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Low-temperature proton exchange membrane fuel cells (LT-PEMFC) have presented themselves as an adequate alternative for future energy conversion systems. However, due to the sluggish reaction rate of the oxygen reduction reaction (ORR), further improvement is needed to reach commercial use. By alloying platinum with the less noble metal, it is possible to obtain nanocatalyst with an improved reaction rate for the ORR and at the same time lower the Pt content. The main issue with Pt alloyed nanoparticles is their instability. We present a novel methodology based on the identical location of the same nanoparticle to gain further insight into the structure-activity and structure-stability properties of nanoparticulate catalysts for ORR. The methodology consists of combining modified floating electrode (MFE) which is designed to test the activity of the electrocatalytic materials on the transmission electron microscope (TEM) grid and a high-resolution TEM imaging of individual nanoparticle before and after electrochemical protocol at the same location. [1] This way, we can obtain atomically resolved structural information of catalytic material and gain insight into the mechanism of dissolution and redeposition of Pt. We present a case study of Pt-Co nanoparticles supported on high surface area carbon that is imaged before and after a standard electrochemical activation protocol. After the computer analysis of before and after images, several degradation mechanisms can be observed at the atomic scale, such as dissolution and redeposition on the specific surface sites.

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O.S.II.16.

Aptamers on surfaces: Making of Perfect Bioreceptors for sensors

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Aptamers, oligonucleotide-based receptors, have been long used as receptor components for various biosensor applications. We will describe our efforts to not only isolate aptamers for challenging small molecule targets, but also to optimize their structures and the conformational changes they undergo upon ligand binding, all in order to optimally interface them with various materials used in biosensors. We will describe a series of collaborative results with metal oxide FETs, graphene, single-wall CNTs, nanoparticles, and gold surfaces, which overall support the argument that aptamers are indeed optimal and general receptors for numerous analytical applications.

O.S.III.1.

Deposition of nanocomposite diamond-like carbon films under dusty plasma conditions

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Modern applications of carbon-based thin films are numerous. The wide range of their utilisation is given by the great variety of structural modifications of carbon materials, which is truly astounding (*e.g.* graphite, graphene, glassy carbon, DLC (amorphous diamond-like carbon), diamond, etc.). In addition, it is possible to further modify the properties of all the above-mentioned thin-film materials by doping with various elements (*e.g.* DLC films doped with silicon, oxygen, nitrogen or fluorine). The DLC films may also be doped by nanoparticles of silver, or other metals (copper, gold, titanium), which are well-known for their antibacterial and antiviral properties. Plasma Enhanced Chemical Vapor Deposition (PECVD) using dusty plasma is an excellent tool for doping the films with nanoparticles.

The aim of the present work was to prepare nanocomposite diamond-like carbon films (NDLC) using PECVD) under dusty plasma conditions.

X-ray Photoelectron Spectroscopy (XPS), Fourier Transform Infrared Spectroscopy (FTIR) and Rutherford Backscattering Spectroscopy (RBS) combined with Elastic Recoil Detection Analysis (ERDA) were used to study the atomic composition and chemical structure of the films. The mechanical properties of the films were studied using nanoindentation technique and the surface structure was studied using atomic force microscopy. The surface properties were studied using surface free energy measurements. The thermal stability of the films was studied using thermal desorption spectroscopy.

The present work is supported by Czech Science Foundation under project GACR 19-15240S.

O.S.III.2

The effect of the biopolimers addition on the stability of emulsions of essential oils

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Essential oils can be used not only in the perfume industry, but their other role is also e.g. repellents. The use of the right composition of oils allows you to achieve the effect of repelling animals only through the smell which is safe for them and if the composition is properly selected, it does not burden the natural environment. A good repellent must, in addition to the main action, release the smell as long as possible and remain on the surface. Its viscosity should be greater than the viscosity of water, which will allow both slowing down the release of the fragrance and longer staying on the surface. As a result of our research, it was found that the best thickener will be guar gum, while the stabilizing polymer is CMC (carboxymethyl cellulose). Chitosan was also used in preliminary studies, and although it did not stabilize emulsion systems sufficiently, it left significant potential for further research. Emulsion systems contained 1-2 % essential oils, 1 % biopolymers and 2 % thickener. The most important was stability testing at 40 ° C, which is related to the process of subsequent use and storage. It was assumed that the finished product will be stored for 40 days. Stability was tested using Turbiscan Lab^{Expert}, this device works in the technique of multiple light scattering. The stability of the emulsion system is obtained by macromolecular and steric stabilization. Turbiscan Stability Index (TSI) coefficient proposed by the turbiscan manufacturer is well suited for analysing the stability of systems of this type.

Acknowlwdgements: The National Centre for Research and Development Project number: POIR.01.01.01-00-0870/17

O.S.III.3.

Processing infrared images as a result of Thermal Non-destructive Testing

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Quick development of constructional composite materials application is caused by their excellent mechanical and strength-related properties, combined with a low specific weight. One of the basic groups of reinforcement materials in composites are fibres. The main reason of defects in structures of composite materials is the variability of working charges in constructions during the process of using. Existed defects are complicated because of the effects like loss of continuity of reinfused fibres, binder cracks and loss of fibres adhesiveness to binder. Diagnostic methods, which are effective with relation to metals became little effective when used in detection of defects in composite materials. This caused greater interest of diagnostic techniques with using infrared thermography. Non-destructive testing via thermographic methods, as well as other test methods, has limitations on types, geometric dimensions, and depth of defect below the surface of tested materials. It is used to process images (thermograms) obtained during experimental testing. In the process of analysing hundreds of images containing details, they are replaced by a limited set of distinct features, prone to use of methods and algorithms for recognition. The examples presented in this paper show the role that thermogram processing can play by using special methods for detecting a defect in tested materials.

O.S.III.4.

D-Xylose dexidration to furfural in presence of H-Beta zeolite in water

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Renewable energy sources will take precedence over non-renewable sources in the future. This is a consequence of high energy requirements and reduced reserves of fossil fuels. The conversion of pentoses and hexoses from lignocellulosic materials leads to valuable compounds such as furfural. Currently, furfural is used as a platform chemical in the chemical industry because it can be converted into many polymers, fuels, *etc.* Heterogeneous catalysts are ecologically more advanced than homogeneous ones, primarily due to the possibility of being reused in the process, and also the processes in which heterogeneous catalysts participate can be continuous. In this work, xylose conversion was investigated over a H-Beta zeolite catalyst in water as a solvent. Xylose was dissolved in 120 ml of deionized water and after that the catalyst was added in a certain mass ratio and stirred. Samples were collected every one hour for 6 hours. Different effects of reaction conditions were investigated such as stirring speed, catalyst mass, catalyst regeneration and concentration of xylose. The advantage of commercial H-Beta zeolite is achieving much higher yields than blank reactions, but it seems that it can also cause degradation of the product. The only product identified in the reaction mixture was furfural with a selectivity of 37 mol % and a catalyst/xylose mass ratio of 3/1 at 160 °C. Lower yields are the consequence of the fact that water is suitable for humins production.

O.S.III.5.

pH-Responsive giant polymeric vesicles prepared via polydimethylsiloxane (PDMS) microfluidics

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Polymeric vesicles (PVs) are self-assemblies manufactured from amphiphilic diblock copolymers. PVs are capable of accommodation of hydrophobic compounds in their membrane and hydrophilic agents in their aqueous lumen. The advantage of PVs is their ability to deliver a protected payload into intracellular environment, stimuli-triggered release, compartmentalization properties, enhanced stability and low permeability (less drug leakage) if compared to liposomes. Herein, we present highly monodisperse pH-responsive giant PVs by water/oil/water (W/O/W) double emulsion method prepared in a sol-gel coated PDMS device with channels selectively modified with polyethylene glycol (PEG). The PDMS devices were fabricated by soft lithography and coated with sol-gel tetraethyl orthosilicate (TEOS)-technique that produced durable glasslike layer, which significantly increased resistance of PDMS. The selected inner junction channels were rendered by the hydrophilic coating with PEG via plasma activation. As pH-responsive polymer the poly[2-(diisopropylamino) ethyl methacrylate-*b*-poly(ethylene-glycol) was synthesized by reversible addition−fragmentation chain-transfer (RAFT) polymerization and used in combination with poly(1,2-butadiene)-*b*-poly(ethylene oxide) for the production of homogeneous pH-responsive giant PVs. The pH-responsive behaviour was studied in detail by confocal microscopy and the results demonstrated the spatial and temporal pH-controlled PVs disruption under simulated relevant physiological conditions. This approach can be utilized to fabricate pH-responsive delivery systems for several active compounds, microreactors, and artificial organelles toward cell mimicking.

This work was supported by Czech Science Foundation (Grant # 20-13946Y and # 20-15077Y).

O.S.III.6.

Electrochemical detection of dihydroxybenzene isomers using carbon supported catalysts

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Simultaneous detection of dihydroxybenzene isomers is an interesting topic in analytical chemistry. The electrochemical detection of the ortho (Catechol-CC), meta (Resorcinol-RS) and para (Hydroquinone-HQ) isomers of dihydroxybenzene using carbon-supported catalysts (Pt on carbon) coated on Screen-Printed Electrodes (SPE) has been investigated. CC and HQ are widely used in various industries such as textiles, plastics, oil refineries, cosmetics, antioxidants, pesticides and pharmaceuticals. They are highly toxic and have been considered as environmental pollutants even at very low concentrations by Environmental Protection Agency and the European Union.

Carbon in different allotropic forms (carbon black, nanotubes, graphene) exhibits good electrochemical activity in the redox processes of CC in acidic media (1 M HCl). Replacing carbon black with single-walled carbon nanotubes resulted in the oxidation peak occurring at a lower potential, down from 0.8 to 0.6 V *vs.* Ag/AgCl reference. The addition of Pt nanoparticles onto the working electrode (20 % Pt by weight) reduces the oxidation potential further, and reduces the separation between the oxidation and redox peaks, improving reversibility. The use of carbon-support improves the electron transfer characteristics of the working electrode due to the high electrical conductivity of carbon, reduces the loading of required Pt by providing a large electrochemical surface area (> 500 m^2 g^{-1}) and is also more resilient to electrochemical oxidation compared to pure Au or Pt electrodes. The Pt nanoparticles decrease the activation energy required for the redox processes by weakening the hydrogen bonds, allowing for the oxidation to occur at comparatively lower potentials and thereby decreasing the electrical stresses on the working electrode, allowing for longer operating cycles. Selective detection of CC and the other isomers (RS, HQ) has been observed by using Differential Pulse Voltammetry (DPV) on the same SPE working electrode with a solution containing all three isomers.

V.O.S.1.

Virtual Offline Lecture

Novel engineered micro-nano structured renders nuclear power among the most ecological friendly technologies

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Actual nuclear power is in its infancy after about one century from the first discoveries, having many issues, from safety, security, non-proliferation politics, and most acute are the cost of energy and fuel cycle that renders it undesirable. As it is well known, the electric light did not come from continuous development of candle technology, and Damascus swords were not possible without Damascus steel, so advanced nuclear power may not be created without advanced nuclear materials and is the turn of engineered nano-hetero materials to make possible a significant advancement in nuclear power, making it cheap, reliable and most ecological friendly power source. All these materials must do is to bring in harmony, the nuclear reactions with the materials hosting these reactions. Five families of engineered micro-nano-hetero materials have been developed in the last 40 years, that are dealing with fission products, transmutation products, neutrons and gamma and knock-on electrons, making possible the creation of a compact solid-state fission reactor with near perfect burning, reducing by two orders of magnitude the ecological impact of the nuclear fuel cycle. It will facilitate the development of fission, fusion and transmutation batteries for advanced applications and production of super-grade isotopic materials.

V.O.S.2.

Virtual Offline Lecture

Characterization of biomaterials used for hip implants

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Hip replacement is a surgical procedure in which parts of the hip joint are removed and replaced with hip implant, made of cobalt-chromium alloy, Ti allloy or stainless steel. This paper aims to provide a comparative analysis of mechanical properties of these three different alloys, focused on their frature and fatigue behaviour, i.e. resistance to cracking. Motivation for such an analysis are failures of hip implants due to static, impact or amplitude loading, *i.e.* fatigue, as shown in Figure 1.

Figure 1. Hip implant fatigue failures

Common mechanical properties, such as tensile and yield strength, elongation, modulus of elasticity and impact toughness are evaluated for all three materials, and presented in a form of comparative analysis. Special attention is paid to the impact toughness testing using instrumented Charpy pendulum, since it enables separation of crack initiation and crack propagation energies. In this way resistance to cracking due to impact loading can be estimated.

Fracture characteristics of Co-Cr alloy, Ti-6Al-4V alloy and stainless steel are also evaluated and compared, both for static and amplitude loading. In the first case, fracture toughness, as the relevant material property, has been measured, whereas in the later one Paris law coefficients are obtained, in both cases by using standard ASTM procedures. Fracture toughness values are then compared to analyse resistance to brittle cracking, whereas Paris law coefficients are used to estimate structural life of hip implants made of different materials. Toward this aim initial crack length is either detected or assumed, while the final (critical) crack length is evaluated from fracture toughness and yield strength values, enabling another comparative analysis of Co-Cr alloy, Ti-6Al-4V alloy and

V.O.S.3.

Virtual Offline Lecture

A new, fast and sustainable method to produce leg material for thermoelectric generators

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The development of renewable energy technology is absolutely essential. Thermoelectricity is a simple technology applicable for direct conversion of heat to electricity (any exhaust heat, geothermal, solar heat or even body heat), applying a thermoelectric (TE) device. For a TE generator p- and n-type legs are needed, which are connected thermally in parallel and electrically in series and should be producible via an easy, fast, cheap and sustainable route. Additionally, they should have a high figure of merit, ZT ($ZT = ST/\rho\lambda$ with S the Seebeck coefficient, T the temperature, ρ the electrical resistivity and λ the thermal conductivity).

Applying severe plastic deformation (SPD) via high-pressure torsion (HPT) we could produce solids from commercial skutterudite powders (p-type: $DD_{0.7}Fe_3CoSb_{12}$ and n-type $(Mm,Sm)_{0.15}Co_4Sb_{12}$). With a custom-built HPT equipment, we produced within 15 to 30 minutes samples with a diameter of 30 mm and a thickness of 1 mm and of 8 mm. Applying this technique, a non-homogeneous deformation with a large strain gradient is introduced, resulting not only in ultra-fine materials, but also in a high density of crystal lattice defects. With such big samples it was possible to study the influence of shear strain on the structural, physical and mechanical properties, but also to measure them orientation sensitive. For comparison a p- and n-type reference sample was fabricated from the same powders applying the traditional method, *i.e.* hot-pressing (HP), which is energy consuming and takes about 4 hours. SPD had no influence on the Seebeck coefficient, and the enhanced electrical resistivity was overcompensated by a much lower thermal conductivity (also after annealing) inducing as net effect an enhanced ZT (~ 1.3 p-type and 0.8 to ~ 2.1 n-type) in comparison to the HP reference sample.

The thick samples, with a weight of about 50 g, showed a rather homogeneous behaviour with ZTs between 1.3 – 1.4 and thermal-electric conversion efficiencies of 12 – 14 % and could be directly cut into legs of a thermoelectric module. Due to grain refinement, hardness is higher for all HPT samples in comparison to the hot-pressed material, with increasing hardness from the centre to the rim; elastic moduli are not affected.

V.O.S.4.

Virtual Offline Lecture

Visible light assisted CH_4 and CO_2 activation during dry methane reforming over Ni/CeO_2 catalyst

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This research investigates the possibility of photocatalytically driven methane CO_2 dry reforming reaction (DRM) over 2wt. % Ni/CeO_2, which is an attractive pathway for production of syngas at low temperatures (<500 °C). TEM analysis revealed the CeO_2 support was rod shaped with approximate length of 100±20 nm and thickness of 20±5 nm. The average nickel crystallite size was 6±2 nm. UV-Vis DRS revealed the bandgap of the catalyst stretching 2.37 eV which means the catalyst can be excited by visible light with wavelength below 523 nm.

Self-sustaining thermocatalytic activity was observed above 355 °C over the Ni/CeO_2, giving a low H_2/CO ratio of 0.13. With increasing reaction temperature to 460 °C, the H_2/CO increased to 0.46. During the combined photo-thermocatalytic experiment over the same catalyst illuminated by 790 mW/cm^2 of white light ($400 < \lambda < 700$ nm), H_2 and CO rates reached 4.7 and 8.5 $mmol/g_{cat}$ min at 460 °C, respectively, which is ~2 times higher compared to the thermocatalytic run at identical catalyst temperature. No methane and CO2 conversion were observed below 350 °C in the thermo catalytic regime, whereas in the photo-thermo catalytic mode, the DRM reaction occurred already at 190 °C. In purely photocatalytic mode at 190 °C, H2 and CO were produced with rates of 0.058 and 0.36 $mmol/g_{cat}$ min. During the combined photo thermocatalytic reforming, a 10-20 % relatively higher H_2/CO ratio was recorded in the entire range of catalyst temperatures (190-460 °C) compared to the thermocatalytic run. Arrhenius plots were used to quantify the effect of illumination on apparent activation energy (E_a) for CH_4 and CO_2, which equalled 125 and 120 kJ/mol in the thermocatalytic mode. The E_{as} were lowered to 30±3 kJ/mol for both CH_4 and CO_2 during the combined photo-thermo catalytic reaction. A change in reaction mechanism during photo catalysis and a substantial decrease in the activation barrier(s) of the rate determining step(s) of the DRM reaction is evident. Further work is in progress to identify the origin of observed catalytic improvement because of illumination. This work confirms the principle of using visible light for remarkably accelerating the low temperature conversion of CH_4 and CO_2 to syngas over Ni/CeO_2 catalyst with a substantially higher H_2 selectivity compared to the thermocatalytic reaction.

V.O.S.5.

Virtual Offline Lecture

Solvent deficient method – Mechanochemically induced synthesis of functional nanomaterials

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Increased demand for advanced oxide ceramic nano-powders is driving the development of more efficient and environmentally neutral synthesis methods. Currently, numerous synthesis methods have different environmental impacts, complexity, and safety issues. Between different synthesis methods, the mechanochemical approach emerged as an environmentally friendly alternative to traditional synthesis routes. This presentation is aiming to provide a brief description of a solvent deficient method as a mechanochemically induced synthesis of oxide nanomaterials. This new approach doesn't require additional solvents for the mixing of the regents, or sophisticated equipment and setup. We are going to present a comparative study of Al_2O_3 [1], CeO_2 [2], $BiFeO_3$ [3], La_2O_3 and $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_3$ (BSCF) nanoparticles synthesis by the solvent – deficient method, followed by the resulting powders microstructure and properties comparison.

Acknowledgements: This research was done in the scope of COST Action CA18112. SZ is grateful for the financial support of the Ministry for Scientific and Technological Development, Higher Education and Information Society of Republic of Srpska (Project 19/6-020/961-45/18).

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Poster Presentations

P.S.I.1.

Utilization of nitrogen doped carbon cryogel for efficient removal of pharmaceutical residues from water

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In this work nitrogen doped carbon cryogel samples (CCN) were tested for removal of pharmaceutical residues (carbamazepine (CBZ), naproxen (NPR), diazepam (DZP) and diclofenac (DKF)) which are recognized as a water pollutant. It is well known that incorporation of different heteroatoms in carbon structure may affect many characteristics of carbon materials sush as increase of specific surface area and surface charge, enlargement of the total amount of surface functional groups as well as formation of some new functional groups. By functionalizing of carbon materials through doping it is possible to improve their adsorption characteristics which was the goal of this work. Structural and surface characterization, as well as analysis of surface chemistry of materials were performed. Kinetics and equilibrium adsorption studies were investigated using a batch experimental approach. pH influence of pharmaceutical solution on adsorption efficiency was also investigated. Pharmaceuticals concentration measurement were analysed using UPLC technique coupled with PDA detector. The results of this work suggests that the carbon cryogel sample with higher concentration of incorporated nitrogen showed a better adsorprion kinetics parameter than other samples. This is in direct connection with higher specific surface area obtained for these samples. Also, presence of nitrogen in the carbon structure obviously affect electronic structure of the material, which led to formation a stronger electrostatic and π-π interaction between functional groups on carbon surface and pharmaceuticals. pH values of solution affect protonation and deprotonation of analytes which is confirmed by better adsorpion in acidic medium. This work provides a new opportunity for efficient removal pharmaceuticals in water treatment.

P.S.I.2.

Mercerized jute fabrics suitable for technical textiles

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Simple chemical modifications by using 17.5 % NaOH (for 5, 15, or 30 min) were applied to obtain jute fabrics suitable for various types of technical textiles such as carpet backing and advanced protective textiles, *i.e.*, protective clothing in environments sensitive to electrical discharges. The raw, as well as mercerized jute fabrics, were characterized in terms of their chemical composition (cellulose and hemicellulose content), structural characteristics (fabric weight, thickness, and porosity), and fibbers' surface morphology (determined by FESEM). In order to assess their ability for utilization as technical textiles, the compression properties (compressibility and compression resilience), abrasion resistance (by determining mass loss after 750 and 1000 cycles), and volume electrical resistivity were studied. The obtained results revealed that with prolonging the mercerization duration from 5 up to 30 min, the hemicellulose content decreased, fabrics' compactness increases contributing to decreased compressibility and increased compression resilience. Concerning the abrasion resistance, a mass loss of about 19 % was observed after 750 cycles in the case of raw jute fabric, while the mercerized jute fabrics possessed up to 7.6 % mass loss even after 1000 cycles. Such behaviour could be ascribed to the higher friction force between the yarns within the mercerized fabrics and between the fibres within the yarns enabling less loss of fibres from the fabric surface. Mercerization for 5 min leads to a decrease, while those performed for 30 min resulted in an increased volume electrical resistivity.

Funding: This work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Contract No. 451-03-9/2021-14/200287 and 451-03-9/2021-14/200135).

P.S.B.I.3.

Oxygen diffusion in doped Ti-Al alloys

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Titanium aluminides are considered as ones of the most promising high temperature structural materials for aero-engine components. They have good combination of mechanical properties; however, the Ti-Al alloys with increased Ti concentration are characterized by an insufficient high temperature corrosion resistance. Growth of mixed oxide scale (TiO_2 and Al_2O_3) on the surface of the Ti_3Al and TiAl alloys is responsible for lower corrosion resistance. Therefore, it is necessary to control the structure and properties of the surface layers in Ti-Al alloys and also the conditions of their oxidation. In this connection it is necessary to understand better the mechanism of surface oxidation of these alloys at the microscopic level. This implies theoretical studies of the interaction of oxygen with a surface and its diffusion from surface into bulk and also in bulk alloys in dependence on their composition. In this work we discuss the oxygen diffusion in bulk Ti_3Al, TiAl and $TiAl_3$ alloys.

Oxygen diffusion properties in the Ti-Al alloys are studied by the projector augmented-wave method within the density functional theory. In order to calculate the oxygen migration barriers along possible paths, the Climbing Image Nudged Elastic Band method (CI-NEB) was used. It was shown that the oxygen prefers mainly the Ti-rich octahedral sites in bulk alloys. The appearance of aluminium in the nearest neighbours of oxygen leads to a decrease of its absorption energy in the set of Ti_3Al–TiAl–$TiAl_3$ alloys. The greater solubility of oxygen in Ti_3Al is connected with existence of octahedron formed by six Ti atoms. We demonstrate that the oxygen migration barriers from preferred absorption sites decrease with increase of Al content in the Ti-Al alloys. As consequence the diffusion coefficient and its anisotropy in the Ti-Al alloys increase with the Al content. Impurity influence on the oxygen absorption and migration energy is investigated. We found that almost all impurities of 4*d* metals and elements of IIIA and IVA groups lower the O absorption energy, if they occupy the Ti-sublattice but impurities on the Al-sublattice have the opposite effect. Transition metals substituting Ti result in a decrease of the migration barriers and an increase of the oxygen diffusivity, whereas the impurities of *p*-elements on the Al-sublattice reduce it.

Support from the Russian Foundation for Basic Research (grant N 18-03-00064_a), ISPMS SB RAS (project III.23.2.8) and Tomsk State University Competitiveness Improvement Program is gratefully acknowledged. Numerical calculations were performed on the supercomputers at TSU and MSU.

P.S.I.4.

Mechanochemical synthesis of TiO_2-CeO_2 powder for the purpose of building an oxygen sensor

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Mixed oxide systems, such as TiO_2-CeO_2, exhibit advantageous physicochemical and electronic properties that are unobserved in their components. This is of great interest in gas sensors research and applications. In this work, TiO_2-CeO_2 powders were obtained by fast and cost-effective mechanochemical synthesis by high energy ball milling. Thick films were deposited on alumina substrates with interdigitated gold electrodes by screen-printing of the paste made out of synthesized mixed oxides. Samples were then thermally treated at 800^{o}C. Various methods of characterization, such as X-ray diffraction (XRD), UV-Visible diffuse reflectance (UV-Vis-DRS), scanning electron microscopy (SEM) and atomic force microscopy (AFM) were used to evaluate the morphological, structural and electronic properties of the prepared materials.
The films made of TiO_2-CeO_2 were exposed to various concentrations of O_2. The electrical resistance of the sensors was measured. With the rising partial pressure of O_2 in a measurement system, resistance was increasing. It was found that TiO_2-CeO_2 mixed oxides synthesized by a mechanochemical process are sensitive to the presence of oxygen in a range of concentrations from 0 to 100 %.

P.S.I.5.

Understanding the photopolymerization and post-processing as a way to enhance thermomechanical properties of 3D printed auxetic structures

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Presented study combines the proper understanding of 3D printing via stereolithography and consequently the 3D printing of auxetic structures with gradient porosity in order to enhance the mechanical response over a broad range of strains and improve the effective energy dissipation. Auxetic structures, considered as one of the 16 smart materials in 21st century, exhibit several enhanced mechanical properties due to the negative Poisson’s ratio. However, the full-scale application of SLA 3D printed smart materials is still limited mainly by the low thermomechanical properties unfulfilling their potential due to the poor understanding of the photopolymerization and post-processing methods. Thus, the main issue was to study the chemical nature of the resin and its crosslink behaviour as well as the printing and post-processing parameters. Herein, we tested a commercial acrylic-based resin undergoing the free radical polymerization, while the variables such as light distribution, printing orientation, specimen thickness and post-curing time was studied with special focus on crosslink density. A model for determining the ideal post-curing time for minimizing the anisotropy in printed bodies which is characteristic for the photo-3D printed bodies, was proposed. It was found that these variables have a large effect on final thermomechanical properties of printed structure. With proper understanding of stereolithographical 3D print and post-processing methods, the properties of final printed body can be improved significantly, enabling fully use the large potential of auxetic structures while being easily scalable by additive manufacturing.

P.S.I.6.

Stability of Pt-based alloy ORR electrocatalysts for PEM fuel cells: Temperature dependent metal dissolution

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Due to the extensive use of fossil fuels and consequently negative impacts on living conditions, the maximum effort should be put into the search for new, renewable energy sources. In this regard, one of the promising technologies are proton exchange membrane fuel cells (PEMFCs), devices in which hydrogen in the reaction with oxygen produces clean electricity and water as the only by-product. The problem of high price and scarcity of widely accepted Pt-electrocatalyst, which is used to overcome naturally sluggish kinetics of oxygen reduction reaction (ORR) at the cathode of PEMFC, is solved by combining platinum with more affordable and less noble 3d transition metals supported on a conductive carbon support. However, there are still some challenges to be addressed in the development of ORR electrocatalysts, where long-term stability is of the utmost importance. Complex degradation phenomena, which can include platinum dissolution and carbon substrate corrosion as the primary degradation mechanisms, as well as the less noble metal dissolution, agglomeration, particle detachment, Pt re-deposition and Ostwald ripening as the secondary degradation mechanisms, are highly dependent on applied potential range. However, since the PEMFCs operate at temperature up to 80 °C, the effect of temperature to the electrocatalyst degradation should be also taken into account. In order to investigate the effects of temperature on dissolution of metals in acidic media (0.1 M $HClO_4$), in-house designed Pt-Co/C electrocatalyst was studied with a combination of two advanced methodologies: the high temperature disc electrode (HT-DE) methodology and the high temperature electrochemical flow cell coupled to an inductively coupled plasma mass spectrometer (HT-EFC-ICP-MS) methodology. Whereas the former enables accelerated degradation tests (ADTs) in liquid electrolyte half-cell by using a standard rotating disc electrode at temperatures relevant to the real operating conditions of PEMFC, the latter allows for precise (ppb range) time-and-potential resolved temperature-dependent measurements of dissolution of metals. The extensive electrochemical characterization as well as the structural characterization that includes X-ray diffraction (XRD) and transmission electron microscopy (TEM), enabled to gain better understanding of temperature impact on the Pt-alloy electrocatalyst stability in terms of metal dissolution.

P.S.I.7.

High entropy materials for electrochemical applications

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In recent years, a new class of high entropy materials has created scientific interest besides the already known high entropy alloys, namely, the “high entropy oxides” (HEOs).1,2 These compounds are based on the concept of entropy stabilization of crystal structures in oxide systems by inserting/embedding multiple metal cations into single-phase crystal structures. The interactions among the various metal cations lead to interesting and often unexpected properties. Some of the compounds show electrochemical and structural properties, which improve the capacity retention of conversion materials for Li-ion batteries.3,4 Another promising material class are the high entropy oxyfluoride systems (HEOFs), showing great potential to be part of next generation cathode materials.5 The modular building approach for these high entropy materials allows tailoring the composition to develop customized electrode materials, *e.g.* with reduced Co content.

In our poster we present different approaches, which utilize the high entropy concept, for novel high entropy electrode materials.3,5 By replacing, adding or subtracting elements, the electrochemical properties can be tailored and the influence of different elements evaluated.

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P.S.I.8.

Resistive Switching Memory Devices based on 2D Halide Perovskites

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Resistive switching memory devices based halide perovskites are emerging as revolutionary data storage devices due to their switching materials (halide perovskites) received considerable attention in recent years. Among the electrical characteristics of halide perovskites, its current–voltage (I-V) hysteresis, which may occur because of defect migration, makes ReRAM employ halide perovskites as switching materials. In general, the halide perovskite means a 3-dimensional (3D) crystal structure with the general formula ABX_3, where a monovalent A^+ cation, a divalent B^{2+} cation, and the 1^- charge of the X halide anion. In the resistive switching process, conductive filaments in the 3D halide perovskite show repeatable formation and rupture. However, as a switching material, the morphology of the 3D halide perovskite film is not uniform, and the ON/OFF ratio of the memory device is low. To overcome these challenges, quasi 2-dimensional (2D) halide perovskites can be applied to the resistive memory devices. The quasi-2D halide perovskite structure formed by inserting into large molecule in a 3D perovskite structure, which means the 3D structures are broken, and become quasi 2D layered structures. Quasi-2D halide perovskites have the general formula $(RNH_3)_2A_{n-1}B_nX_{3n+1}$ ($n = 1, 2, 3, \ldots$), where RNH_3 is a large organic cation such as a large aliphatic or aromatic alkylammonium cation. Thus, as the n-values decrease, the dimensionality of halide perovskites changes from 3D to quasi-2D and 2D structures.

Herein, we apply quasi 2D layered halide perovskite in resistive switching memory devices. This research will contribute to the improvement of switching behaviour of memory devices and the better understanding on the resistive switching mechanisms based on the quasi-2D layered halide perovskites.

P.S.I.9.

Electrochemical control of magnetism: on the conversion of hydrated FeF_3 with Li to Fe and LiF

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Utilizing the concept of Li-ion batteries (LIBs), where active materials are reversibly de/lithiated over thousands of cycles and show distinct redox reactions depending on the applied potential.[1,2] As, Conversion-type electrode materials are prominent examples of potential Li-ion battery cathodes and/or anodes with large specific capacities. Conversion reactions often rely on complete reduction or oxidation of a transition metal, leading to multi-electron redox processes per formula unit, accompanied by changes of crystal structure and electronic configuration.[3,4] Consequently, of materials properties such as magnetization. Here, we report on the utilization of the FeF_3/Fe conversion reaction to reversibly control the magnetization. Hydrated FeF_3 was chosen as electrode material and the changes in magnetization upon reversible redox reaction against Li counter electrode monitored by means of Superconducting Quantum Interference Device magnetometry. In situ measurements provide insights into the changes in magnetization occurring during the conversion reaction, specifically revealing the transition from paramagnetism to ferromagnetism.[5]

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P.S.I.10.

Electrical properties of epoxy composites based on carbon black and multi-walled carbon nanotubes

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This work is devoted to investigation of electrical properties of epoxy composites based on carbon black (CB) and multi-walled carbon nanotubes (MWNTs). The carbon fillers were investigated using transmission electron microscopy, energy dispersive X-ray spectroscopy, particle size analysis, etc. Epoxy/CB/MWNTs and epoxy/CB composites with various loadings were obtained. AC electrical properties (20 Hz – 1 MHz) were measured. The content of CB in the composites was ranged from 0 to 5 wt.% and for MWNTs it was 0–0.025 wt.%. It was found that relatively small addition of MWNTs into epoxy/CB composite induced an increase in conductivity and permittivity. For a permittivity at low frequency, the addition of small loadings of MWNTs made it possible to increase its values by several orders of magnitude. A comparison of the electrical properties of pure MWNTs and CB with the epoxy/CB/MWNTs and epoxy/CB composites was carried out.

P.S.I.11.

Increasing catalytic activity of molybdenum disulfide for hydrogen evolution reaction

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Different catalysts for hydrogen evolution reaction have been the subject of scientific research in recent years. Considerable attention has been given to molybdenum disulfide due to its tunable electronic properties and layered structure with catalytically active edge sites. For improvement of both catalytic and photocatalytic activity of material, elemental doping and structural modification of material are commonly used as effective approaches to change the surface properties and band structure. Dopant ions and defects can be induced in structure by low energy ion beam irradiation. Depending on ions energies and fluences different interactions are possible: production of vacancies, dislocations, deposition of incident ions which all cause changes in properties of the catalyst. In present work molybdenum disulfide was synthesized via hydrothermal synthesis route and obtained powder was irradiated with carbon and hydrogen ions. Ions energies of 20-40 keV and fluences of 10^{14}-10^{17} ions/cm^2 were used. Synthesized powder is composed of spherical, flower-like structures consisting of nanosheets petals. The X-ray diffraction patterns confirm hexagonal type of structure, while Raman spectroscopy reveals Mo-S in-plane and out-of-plane vibrational modes. Catalytic and photocatalytic properties for hydrogen evolution are investigated with impedance spectroscopy, linear sweep and cyclic voltammetry. All measurements are performed in an acidic electrolyte solution (0.1M H_2SO_4) at room temperature. Irradiated samples show enhanced hydrogen evolution compared to the as-prepared sample. Decrease up to 100mV of potential required to achieve a current density of 10 mA/cm^2 can be observed. With illumination this potential is decreased by another 20 Mv.

P.S.I.12.

Investigation of thermodynamic parameters of high concentration alkaline activators in the geopolymerization process of metakaolin

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Alumino-silicate materials are environmentally friendly in terms of energy efficiency and low energy consumption for synthesis. The synthesis of such materials implies a reduction in the production of greenhouse gases, ie CO2. In order to optimize process of geopolymerization, the investigation of thermodynamic parameters of alkali activators are important. In this paper, the thermodynamic characteristics (density, refractive index and sound velocity) of homogeneous solutions of alkaline activators are examined over the temperature range 15-60°C. Porous silicate materials were synthesized from, an alkaline activator consisting of a solution of NaOH of different concentrations (10M-16M NaOH) and sodium silicate. Four series of geopolymer samples GP10M to GP16M were synthesized using the constant ratio of solid and liquid phase. Based on the obtained results thermodynamic properties has been selected to predict the properties of synthesized materials. As the concentration of NaOH increases, the dependences of density, refractive index and speed of sound as a function of temperature become more linear. Also, with increasing temperature, the density values decrease, but the trend is more linear. The chemical composition of metakaolin and the synthesized materials were performed by X - ray fluorescence analysis (XRF method). X-ray diffraction analysis (XRD) as well as Raman spectroscopy were used to identify the phases, monitor the crystallite size as well as the proportion of the amorphous phase in the synthesized porous silicate material.

P.S.I.13.

Morphology and mechanical properties of the nanotubular oxide coating formed on the ultrafine-grained Ti-13Nb-13Zr alloy

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Behaviour of the metallic biomaterials is also regulated by surface properties, which is an important factor in interactions of the implant material with the surrounding tissue. The lower value of modulus of elasticity and closer to that of a bone is one of the crucial surface properties in accepting the implant material from the surrounding tissue, and reduces the possibility of slow disappearance of bone in contact with the implant. In the present study, nanotubular oxide layer on Ti-13Nb-13Zr alloy (coarse-grained (CG), and ultrafine-grained (UFG), obtained by high pressure torsion (HPT)) alloy was formed by means of electrochemical anodization in the 1M H_3PO_4 + NaF electrolyte, during 60 and 90 minutes. The scanning electron microscopy (SEM) was used to characterise the morphology of the surface. It was shown that the nanotubular oxide layer was obtained using the electrochemical anodization process during both anodizing times. The aim of this study was to determine the nanomechanical behaviour of the surface - modulus of elasticity and nanohardness, of the CG Ti-13Nb-13Zr and UFG Ti-13Nb-13Zr alloys before and after electrochemical anodization process, using the nanoindentation technique. The displacements during nanoindentation tests were 2000 nm for non-anodized samples and 10 % of the thickness of nanotubular oxide coating for anodized samples. Loading-displacement curves were obtained during the nanoindentation tests. Each curve consists of the loading part, the dwell period at the maximum load of the indentation and the unloading part and they use for determinate maximum mean values of load on the samples and the presence the surface deformation. Also, in order to characterise deformation of the nanotubes after nanoindentation SEM was done. Obtained results showed that surface of the anodized alloys had lower modulus of elasticity than surface of the non-anodized alloys, which means that the values are closer to those of bones, making the discontinuity of mechanical properties at the bone-implant interface less pronounced. The nanoindentation test showed that surface of the anodized UFG alloy had the lowest modulus of elasticity of the surface than all tested samples, which makes it more acceptable for biomedical usage.

P.S.I.14.

Optimization of *in vitro* conditions for 3D culture of rat glioma cells

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Cancer is the second leading cause of death globally, making the search for its cure one of the most important challenges of the 21st century. With ethical questions regarding animal testing and inconsistency of results of cancer drug testing in standard two-dimensional (2D) monolayer cell cultures with the results *in vivo*, there is a pressing need for better *in vitro* models of human cancers that will provide more relevant systems for cancer drug screening. Three-dimensional (3D) *in vitro* systems based on natural polymers with immobilized cancer cells that mimic cancerous tissue and bioreactors that provide relevant chemical and physical signals could close the gap between 2D *in vitro* and *in vivo* cancer models. The aim of this study was to optimize culture conditions for the rat glioma cell line C6 immobilized in alginate microfibers in perfusion bioreactors in terms of cell density and perfusion rate. In this study we investigated following sets of parameters: perfusion rate of 0.12, 0.25 and 0.30 ml min^{-1} coupled with the cell density of $4\cdot10^6$ cells ml^{-1}, and perfusion rate of 0.30 ml min^{-1} coupled with the cell density of $8\cdot10^6$ cells ml^{-1}. Microfiber cultures under static conditions in Petri dishes served as controls. The results have shown that the perfusion rate of 0.30 ml min^{-1} in combination with the cell density of $8\cdot10^6$ cells ml^{-1} yields higher cell viability and proliferation compared to the control static culture. These results indicate the importance of culture medium perfusion in the bioreactor for improved mass transfer of nutrients and oxygen to alginate microfibers so that the investigated system shows potentials for use as a model system in cancer research.

P.S.I.15.

A Possible Approach In Wound Management – An Exfoliated Hydrogel Layer, Based On Polysaccharide Gum Karaya Modified With Carboxymethyl Cellulose, Covered By Natural Hydrophobic Layer

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In the focus of this research, an exfoliated layer is made with various functions to advance the treatment of skin wounds, as well as to support the function of widely used primary dressings applied to the wound bed. Correspondingly to the type of the wound, effective treatment is still facing many limitations: mainly inflammation, desiccation, and scar formation.

Here, a freeze-dry process is used to make the hydrogel layer of blending solutions of polysaccharides, based on Gum Karaya (GK) and Carboxymethyl-cellulose (CMC) and specific substances, called enzybiotics, targeted against methicillin-resistant *Staphylococcus aureus.* The hydrophobic cover placed on the top of the hydrogel layer is based on the emulsification of a certain oil into a elastic structure and freeze-dried.

The hydrogel layer is used for hydration due to the presence of high water absorptive CMC. GK can remove emergent necrotic tissue and the added antibacterial enzymes are directly released into the wound bed and prevent inflammation. To sheet the hydrogel layer and prevent water evaporation, the hydrophobic cover is used. Here, an additional value of natural oil components is believed to eliminate scaring and repairing the skin's lipid barrier function. The layers composition provides oxygen support, and its non-adherent property allows painless remove. Multiple changing will fight extensive inflammation and it simply creates non affecting conditions for the cells to start regeneration processes that occur inside any primary dressing layer. The layer is evaluated with questions that lead to its biocompatibility - morphology, elasticity, hydrating capacity, adhesivity, oxygen permeability, antibacterial properties, and cytotoxicity. In the case of hydrophobic layer, its potence to incorporate oils into the structure.

Cheap and easy obtainable, biocompatible materials are believed to move the effectiveness of surgical treatment towards better outcomes.

P.S.I.16.

Pro-healing protein release from 3D-printed „smart“ hydrogel carriers applicable in regenerative medicine

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In recent years, there has been an increase in the use of 3D printing technologies in regenerative medicine to produce medical implants. This work deals with the 3D printing of a hydrogel carrier based on itaconyl-modified PLGA-PEG-PLGA thermosensitive copolymer,[1] which can be crosslinked with blue light in the presence of a water-soluble nontoxic photoinitiator.[2] The copolymer for 3D printing is water soluble, and bioresorbable in the human body. The printing process was performed by direct ink writing method at ambient temperature between 20-40 °C to avoid bioactive substances damage (*e.g.* growth factors) incorporated into the copolymer water solution before the printing process.

A thermostable 9-point mutant of fibroblast growth factor 2 (FGF2-STAB®, Enantis L.t.d.) was chosen as the ideal bioactive component for its ability to support the growth and the formation of new vessels (angiogenesis), leading to improved wound healing, tissue regeneration and contributes to the pathogenesis of several diseases (cancer or atherosclerosis).

This work was focused on the FGF2-STAB® protein release monitoring of from a 3D printed hydrogel matrix. The effect of the copolymer degradation at physiological solution on the amount of released protein was monitored by various methods, namely UV-VIS spectrophotometry and SDS-page electrophoresis. The release kinetics and changes between the different modification of used materials were monitored. Based on the results one-step first-order release kinetic was observed.

Acknowledgement: Grant Low temperature 3D printed bioresorbable hydrogels as carriers of pro-healing protein for tissue regeneration is realised within the project Quality Internal Grants of BUT (KInG BUT), Reg. No. CZ.02.2.69 / 0.0 / 0.0 / 19_073 / 0016948, which is financed from the OP RDE. The authors greatly appreciate the collaboration with Enantis, s.r.o., which provided the stabilized protein FGF2-STAB® for this project. All rights reserved.

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P.S.I.17.

Viscoelastic properties of resorbable PLGA-PEG-PLGA based bioinks for additive manufacturing technology in regenerative medicine

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Additive manufacturing technologies have been getting very popular in the field of regenerative medicine to fabricate various resorbable implants, carriers for control drug delivery, or wound covers. In this work, PLGA-PEG-PLGA based hydrogels were studied as a very promising material for low-temperature extrusion-based 3D printing of hydrogel scaffolds. PLGA-PEG-PLGA is an FDA-approved, biodegradable, and bioresorbable copolymer[1]. Furthermore, the PLGA-PEG-PLGA thermosensitive copolymer can be modified by itaconic anhydride with reactive double bonds and carboxylic acid groups, and then itaconyl-modified PLGA-PEG-PLGA can be crosslinked by irradiation using harmless blue light in the presence of water-soluble nontoxic photoinitiator[2]. Moreover, low temperature during the printing process allows the hydrogel to be enriched with therapeutic biomolecules such as drugs, proteins, or growth factors to enhance tissue regeneration. Since the 3D printing technology requires perfect printability and cohesion, the rheological properties are crucial parameters. However, several studies on PLGA-PEG-PLGA hydrogel rheology have been introduced[3,4], in this study, the hydrogel was modified to be crosslinked via blue light as well as the proteins were added. Therefore, the effects of hydrogel concentration, crosslinking time (irradiation time), and protein addition on the viscoelastic properties were investigated using rotational rheometer. Lysozyme (14 kDa) and albumin (67 kDa) were chosen as the model proteins for this study. One can say the high concentrated hydrogels (30 wt.%) are the most optimal for the printing of porous scaffolds unlike low concentrated hydrogels (20-25 wt.%) which are more suitable to print unporous films with define and regular thickness.

Aknowledgement: Grant Low temperature 3D printed bioresorbable hydrogels as carriers of pro-healing protein for tissue regeneration is realised within the project Quality Internal Grants of BUT (KInG BUT), Reg. No. CZ.02.2.69 / 0.0 / 0.0 / 19_073 / 0016948, which is financed from the OP RDE.

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P.S.I.18.

Synthesis, characterization and possible application of bacterial cellulose-ceria composite

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Bacterial cellulose (BC) is a promising natural polymer with a range of characteristics such as biocompatibility, microporosity, transparency, conformability, elasticity, the ability to preserve a moist environment, as well as absorb exudates in wounds. That is why BC is an attractive material in biomedical applications, especially in skin tissue repairing, but its lack of antimicrobial activity limits its performance. To overcome this shortage, BC was combined with cerium (IV)-oxide (CeO_2) nanoparticles. Series of bacterial cellulose-CeO_2 (BC-CeO_2) composite materials were prepared by soaking bacterial cellulose in different concentrations of cerium-oxide nanoparticle water suspensions. All composites had antibacterial activity, and toxicity, as well as genotoxicity of BC-CeO_2, had been examined. The BC-CeO_2/0.1M composite stands out as it did not show the cytotoxic, nor the genotoxic effect on peripheral blood lymphocytes, and additionally protected the cells from the genotoxic effect in H_2O_2 treated cultures. Redox parameters in blood plasma samples were concentration and time-dependent for PAB and LPP assay. The results of the survey imply that BC-CeO_2 nanocomposite might be a promising wound healing material.

P.S.I.19.

Hydroxyapatite based inserts in restorative dentistry: Effects of calcium substitutions on the bonding ability

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Restorative materials currently used in dentistry have a high failure rate and relatively short lifespan, especially in the case of large cavity restorations. Moreover, a common layer-by-layer clinical procedure in restorative dentistry is time-consuming and allows air bubbles to be trapped in the restoration, which weakens the mechanical properties and eventually results in restoration failure.

The utilization of dental inserts based on hydroxyapatite – the main inorganic constituent of human bones and teeth, would not only simplify the procedure in the clinical protocol but would also improve the biological response of the tissue as well as mechanical properties of the restoration. Natural calcium hydroxyapatite present in dentin structure has a variety of dopants such as Mg, Sr, Fe, Zn, which play an important role in the formation and remineralization of the dentin.

This study aimed to investigate the effects of single and bi- dopant calcium substitutions in hydroxyapatite structure on the bonding ability of dental inserts with a restorative material commonly used in practice. Nanostructured hydroxyapatites doped with Mg, Sr and Mg+Sr were obtained hydrothermally and pressed into cylindrical compacts which were further sintered at 1200 °C. The restorative material used was Filtek Z_250 composite applied with Single Bond Universal adhesive (SBU_Z250). The bonding ability of inserts with SBU_250 was tested using the Shear Bond Strength (SBS) test. The dopants were shown to have a great impact on the phase composition of thermally treated hydroxyapatite, thus on the solubility and mechanical properties of dental inserts, which resulted in different bonding ability with SBU_250.

P.S.I.20.

Poly (methacrylic acid)/gelatin/hydroxyapatite composite hydrogels for bone tissue engineering

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Hydrogels represent three dimensional, hydrophilic, cross-linked networks made of synthetic or natural polymers. Properties such as high water content, biocompatibility and porosity make them attractive for a wide range of biomedical and pharmaceutical applications. However, the soft nature of hydrogels makes them unsuitable for load-bearing applications. In addition, lack of bioactivity prevents complete integration of implant with surrounding tissue. Therefore, by combining hydrogels and different inorganic fillers it is possible to synergize desirable properties of single phases into the resulting composite material. In this work, we synthesized composite hydrogels based on interpenetrating network of poly (methacrylic acid) (PMAA), gelatine and nano-structured hydroxyapatite (HA) for bone tissue engineering applications. Different amounts of HA were incorporated in order to increase mechanical and biological properties of composites. Composites were characterized by SEM, mechanical testing and swelling behaviour. *In vitro* drug release behaviour was investigated in simulated body fluid at 37 °C. The increase in HA amount led to proportional improvement of mechanical properties as well as slower swelling kinetics, which also affected the drug release kinetics.

P.S.I.21.

Wettability of polysiloxane-CNTs composite coatings deposited on glass supports activated by cold plasma

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Plasma modification becomes a more and more popular technique because surface properties of various materials play a key role in its applications. It can be applied for modification and functionalisation of the surface of any materials because during the process only the top layer of a material is treated [1]. Moreover, carbon nanotubes (CNTs) have become also an interesting material because of their numerous use in various fields nowadays. It was proved that adding a small amount of multi-walled carbon nanotubes (MWCNTs) can improve the polymer, among others, its mechanical and electrical properties.

The aim of the study was the comparison of wettability of the nanocomposite coatings deposited on the plasma modified glass supports. The substrates were produced as follows: glass plates were activated by air or argon cold plasma and then they were dip-coated in the suspension prepared by the acid-assisted tetraethoxysilane hydrolysis in the presence of multi-walled carbon nanotubes obtained by the catalytic chemical vapour deposition (CCVD) using pyrolysis of propylene on complex metal oxide catalysts [2] followed by modification with poly(dimethylsiloxane). The wettability of the obtained coatings was examined by the contact angle measurements using the sessile drop method.

It was found that the substrates are hydrophobic – the highest equilibrium contact angle amounted to above 100 degrees.

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P.S.I.22.

Compacted carbon nanomaterials and their conductivity

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In this work, the electrical properties of compacted carbon nanomaterials, such as carbon nanofibers (CNFs), multi-wall carbon nanotubes (MWNTs), were investigated. Carbon nanomaterials were investigated using transmission electron microscopy, Raman spectroscopy, X-ray diffraction, particle size analysis, etc. The powders of pristine CNFs and MWNTs were compacted under pressure (11 MPa) into cylindrical-shaped samples with a diameter of 10±0.2 mm. It was found that it is not possible to obtain the compacts from CNF samples without adding a binder. Therefore, thermally expanded graphite (TEG) was used as a binder. It was possible to compact CNFs with TEG in a ratio of 80:20, 70:30, 60:40 (wt. %). Samples of MWNTs were obtained without adding a binder. The electrical properties were measured in a frequency range from 50 Hz to 1 MHz. For compacted systems CNFs/TEG with mass ratio 60:40, 70:30, 80:20 conductivity decreased from 25 to 5 S/m, from 23 to 6.5 S/m, from 13.4 to 3 S/m when increasing temperature from 30°C to 100°C, respectively. Reducing the amount of TEG addition in the CNFs/TEG system led to a narrowing of the range of variation in conductivity. It was found that heating has a greater effect on CNFs/TEG systems compared to MWNT samples that in turn may be related to the electronic characteristics of the materials.

P.S.II.1.

Structural characterization of TiO_2/CNTs nanocomposites aimed for incorporation in facial masks

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Last year, the health protection of the people from various viruses, bacteria and other tiny pollutants submicron scale has become extremely important all over the world. Due to the growing field of nanotechnology, and extra-ordinary sorbent properties and capturing efficiency of nanostructures as well as the ability to produce nano-fibers with the dimensions of less than 100 nm, new methods can be used to develop protective masks and filters that can remove tiny pollutants and impurities even at nano-metric or submicron scales. Carbon Nano Structures –CNs and their nanocomposites in polymer nano-fibers are among the most important types of nanostructures for this purpose. In this work, we present the structural characterization of TiO2/CNTs nanocomposites aimed for incorporation in facial masks.

TiO_2/CNTs nanocomposites were prepared by simplified sol-gel method and further thermal treatment at 400 ^oC. Variation of different type of CNTs (activated MWCNTs and as prepared SWCNTs) as well as the variation of the content of MWCNTs (20 and 30 % CNTs), and their influence on the structural properties of TiO_2 were studied. The applied instrumental techniques such as XRPD, Raman spectroscopy and thermal (TG, DTA and DTG) analysis points out on achieved interaction between TiO_2 and incorporated CNTs. Morphological changes, observed from the SEM micrographs, revealed better inter-locking of the TiO_2 matrix with SWCNTs than with MWCNTs. Formation of a more structurally disordered and non-stoichiometric anatase phase seemed to be a preferred choice for the obtained TiO_2-CNT nanocomposites for further utilization in nanofibers for incorporation in facial masks.

P.S.II.2.

Densification of boron carbide under high pressures and temperatures

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Additive-free boron carbide (B_4C) powders were densified by using high-pressure “anvil-type with hollows“ apparatus at the pressure of 4 GPa in the range of 1500-1900 °C. The boron carbide ceramics prepared by this method showed a micro-hardness of about 35 GPa, which is very close to the micro-hardness of mono-crystal boron carbide. The compacts were characterized using Transparent electron microscopy (TEM), Scanning electron microcopy (SEM) and X-ray diffraction techniques (XRD). TEM study showed that the grains of boron carbide possess uniformly grain size and no grain growth was observed in the sintered materials. Microstructure of obtained B_4C ceramics depict the present of porosity depending on sintering temperature. The results of this study show that the high-pressure sintering can be a very effective low-temperature densification method for the obtainment of additive-free B_4C ceramic. More ever, the process can be up-scaled for producing large size (16 mm diameter) composites required in various cutting tools and other application in extreme conditions.

P.S.II.3.

Detection of Glyphosate by Surface-Enhanced Raman Spectroscopy

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Glyphosate is one of the most commonly used pesticides on global basis. It is used for the control of weed growth, but it is proven that it can persist in the environment. There are numerous studies indicating its harmful effects on human health. In this work glyphosate is detected by surface-enhanced Raman scattering (SERS) which is an effective technique for detection of various analytes in low concentration. The SERS substrates used for glyphosate detection were silver and gold nanoparticles (NPs). Samples were analysed using 532, 633 and 785 laser excitations. As already reported in the literature, Raman and SERS spectra of glyphosate strongly differ. Here, rather different glyphosate SERS spectra are also obtained using different colloidal solutions and laser excitations. For example, at 532 nm excitation with Ag NPs two prominent SERS glyphosate peaks are at 771 cm^{-1} (which can be assigned to P-C vibrations) and 1052 cm^{-1} (which can be assigned to PO_3 and C-N vibrations). Using Au NPs and 633 nm excitation, the most prominent peaks are at 1024 cm^{-1} (probably assigned to CN or PO_2 and OH modes) and at 1313 cm^{-1} (CH_2 and CC modes). Au colloidal solution and 785 nm excitation resulted in spectra where the most pronounced peak is at 1019 cm^{-1} (doublet). From the SERS spectra it is obvious that the concentration-dependent calibration curve follows a Langmuir adsorption isotherm (the peak intensity is at maximum value when the analyte forms a monolayer on NPs surface). Although glyphosate has a low affinity to the metal surfaces the results suggest different ways of its absorption to the Au and Ag NPs. In this work it was possible to detect glyphosate in solutions of approximately concentrations of 100 nM.

Acknowledgment: This work has been supported by the Foundation of the Croatian Academy of Sciences and Arts.

P.S.II.4.

High Torsion Pressure effect on cast and wrought technical grade pure magnesium

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The paper is focused on the development of the microhardness of commercially pure grade magnesium in two distinct forms (wrought and cast) under the high torsion pressure technology. The high torsion pressure technique is part of the severe plastic deformation group. The material is subjected to very high torsion. The sheer pressure could at standard atmospheric conditions create cracks in the material. Therefore, this process is under constant quasi-hydrostatic pressure, which stops incubation and propagation of the cracks. This creates intense dislocation density inside the material, which leads to the creation of new grain boundaries. This technology, therefore, allows us to influence the grain size of the material and corresponding mechanical properties. The main focus of this article is the evolution of microhardness and microhardness maps on the axial cut of the sample. The effect of several rotations is then evaluated. The microhardness evaluation is then supported by a three-point bend test evaluation of the elasticity module. Furthermore, the evolution of structure was observed using light microscopy. The grain size was then evaluated using EBSD. The grain refinement is more prominent in the casted material where from 1330 µm (as received) the grain was refined to 2.4 µm just after 1/8 rotation. For the wrought material, the refinement was from 19 µm of as received to 2.5 µm after 1/8 µm. The Micro-Hardness profile of the axial cut sample did not show any significant tendency of increase towards the outer edge of the sample. The hardness maps after 1/8 of rotation show the number of standalone peaks at seemingly irregular places. The most intensive increase in the hardness was in both cases observed after 1/8 rotation (about 14 HV0.2 for cast and 11 HV0.2). Furthermore, rotations did not increase the hardness in such a magnitude. The response of material near the indents shows significant plasticity in as-received material compared to HPT processed samples. Interestingly with an increase in rotations, the average microhardness starts to decrease a little (by 3 HV0.2). This is however as seen from maps mostly by decreasing local spikes in microhardness which are observed after 1/8 of a rotation. The yield stress shows similar results to the average hardness. Both cast and wrought samples show an increase after 1/8 of rotation. After 1 rotation they show slight decrees and with further increase of rotations the value of yield stress remains leveled.

P.S.II.5.

Highly hydrophobic self-assembled monolayers on aluminium – carboxylate vs. phosphonate

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High hydrophobicity of an aluminium surface is a key feature to improve its anticorrosive, anti-icing, and self-cleaning properties. Conventionally, wettability of the aluminium surface is modified by increasing its roughness in anodization or zincation process. To further enhance the structural effect, self-assembled monolayers (SAMs) may be formed on the treated surface [1-3]. Although such a procedure enables fabrication of superhydrophobic aluminium surfaces, it is complex and time-intensive. In our work, we investigate the possibility of creating highly hydrophobic SAMs' coatings on the surface of a thin aluminium layer on silicon, prepared using standard thermal evaporation process. We modified aluminium film with aliphatic carboxylic and phosphonic acids to investigate the influence of the head group on the properties of the final monolayer. Using spectroscopic methods (IRRAS, XPS) and contact angle measurements, the structure, stability, and wettability of SAMs was studied. Obtained SAMs show higher contact angle than reported before for this class of molecules on unstructured aluminium surface [4]. We demonstrated, with AFM measurements, that such a wettability discrepancy might arise from increased roughness of our aluminium surfaces. Moreover, we further improved SAMs hydrophobicity by employing fluorinated molecules which resulted in approaching the limit of superhydrophobicity. As a result, we propose a simple method to create highly hydrophobic coatings that may be easily applied to many substrates.

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P.S.II.6.

Degradation of textile dyes by Oxone® activated by cobalt supported chitosan-derived carbon-smectite catalyst

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Chemical degradation by activated Oxone® is one of the most attractive advanced oxidation processes (AOPs) for the treatment of various pollutants including toxic azo dyes. However, the development of an effective heterogeneous catalyst for activating Oxone® is still challenging. In this work a novel cobalt supported carbon-smectite catalyst (Co/cC-S) was prepared through a two-step synthesis. First, the incipient wetness impregnation method was used for the cobalt species to be introduced into chitosan-smectite biocomposite. The impregnated sample was then carbonized in a tube furnace at 400 °C in a nitrogen atmosphere for 1h. The obtained catalyst was characterized using FTIR spectroscopy and low temperature N_2 physisorption. The Co/cC-S catalyst was tested as peroxymonosulfate (in the form of Oxone®) activator in the degradation of two textile dyes, Acid orange 10 (AO10) and Basic Blue 41 (BB41), from their single component and two component aqueous solution. As the first step in catalytic degradation of dyes, decolorization was monitored using UV-Vis spectrophotometry (λ_{max}=478 nm and 605 nm, for AO10 and BB41, respectively). The results showed that Oxone**®** alone is ineffective in the degradation of both dyes. The combination of Co/cC-S and Oxone**®** significantly improved their degradation. The investigated catalytic process at 30 °C in the single component dye solution was very fast for AO10 and somewhat slower for BB41. The AO10 decolorization from the two-component solution was as fast as from the single component solution. On the other hand, the degradation efficiency for BB41 substantially decreased when two dyes co-existed. This result suggests that Co/cC-S activated Oxone**®** exhibited a relatively high priority for attacking AO10. Co/cC-S showed to be a promising peroxymonosulfate activator in the catalytic treatment of wastewaters containing textile azo dyes.

Acknowledgement: This work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Contract 451-03-9/2021-14/200026)

P.S.II.7.

Spectroscopic characterization and redox behaviour of electroconducting poly(p-ADPA) synthesized by simple and eco-friendly method using magnetite nanoparticles as a catalyst

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The investigations of *para*-aminodiphenylamine (p-ADPA) and its polymerizations are of particular interest as p-ADPA is one of the intermediate products (dimer) occurring during the oxidative chemical polymerization of aniline to electroconductive polyaniline (PANI) [1]. Also, p-ADPA has lower oxidation potential than aniline and is much more easily oxidized using weaker oxidizing agents such as hydrogen peroxide (H_2O_2).

Here, p-ADPA is oxidized using an eco-friendly approach with H_2O_2 as the main oxidant and a very small amount of ammonium peroxydisulfate added for efficient initiation, in the presence of magnetite (Fe_3O_4) nanoparticles (NPs) as a catalyst. The synthesized polymeric product, poly(p-ADPA)/Fe_3O_4, is a powder of dark green colour indicating its high conductivity, which was measured to amount $1.8\cdot10^{-2}$ $S\cdot cm^{-1}$ for optimized reaction conditions. This is one of the highest electrical conductivities for the products of p-ADPA oxidations reported in the literature so far, which is comparable with the conductivity of PANI prepared recently by the same approach using Fe_3O_4 NPs and H_2O_2 [2]. FTIR and Raman spectroscopy measurements of the poly(p-ADPA)/Fe_3O_4 powder indicated the presence of PANI emeraldine salt (ES)-like structures with characteristic strong spectral bands attributed to delocalized polarons. Redox behaviour of poly(p-ADPA)/Fe_3O_4 was investigated by means of cyclic voltammetry in 1 M HCl solution. Cyclovoltammograms showed two slightly merged redox peaks corresponding to the interconversion between nonconducting leucoemeraldine base and ES-like form, and the interconversion between ES and fully oxidized pernigraniline salt-like form.

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P.S.II.8.

Magnetic characteristics of nanocrystalline electrodeposit of $Ni_{86.0}Fe_{9.8}W_{1.3}Cu_{1.9}$

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A nanocrystalline powder of $Ni_{86.0}Fe_{9.8}W_{1.3}Cu_{1.9}$ is obtained by electrodeposition from a citrate solution at the current density of 400 $mAcm^{-2}$. The powder particles are of a cauliflower and dendritic shape. They are composed of nanocrystals of the FCC phase of the solid solution of Fe, W and Cu in Ni, captive in an amorphous matrix. As-obtained powder is thermally stable up to 160 °C. In the temperature range from 160 °C to 460 °C the structural relaxation occurs. The cooled powders, after the structural relaxation, have the higher magnetic permeability, lower loss of the active power and lower coercive field. At temperatures above 460 °C, the amorphous phase is crystallizing, and crystal grains of the FCC phase are growing, which results in a decrease of the magnetic permeability, an increase in both the power loss and power of the coercive field.

P.S.II.9.

The effect of grinding time, pressing and sintering of the powders 16 % Fe_2O_3, 4 % $BaCO_3$, 80 % $BaTiO_3$ on the morphology, microstructure, magnetic and electrical properties

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XRD, TEM and SEM analyses show that the composition, phase structure, morphology, magnetic and electrical properties of the as obtained, pressed, and sintered samples depend on the grinding time of the powder mixture 16 % Fe_2O_3, 4 % $BaCO_3$, 80 % $BaTiO_3$. With increasing the grinding time, smaller particles with finer nanocrystals and larger both the density of chaotically distributed dislocations and inner microstrains are obtained. With increasing the grinding time, the magnetization of the pressed samples increases, reaching the maximum at t = 150 min and subsequently decreases. Annealing of the pressed samples in the temperature range from 450 to 650 ºC results in the increased magnetization. After annealing for 10 min at 540 and 600 ºC of the pressed samples, obtained from the powders ground for 150 min, their magnetization at 25 ºC was 17 and 62.5 % respectively, higher than magnetization of unannealed samples. The magnetization of samples pressed and sintered for 2 hours at 1200 ºC also depends on the grinding time. The magnetization of the sintered sample, obtained from the powder ground for 150 minutes was for 209% higher than that of as-pressed sample. The magnetization of the sintered samples obtained from the powders ground from 30 to 150 min, annealed for 10 minutes at the Curie Temperature T = 550 ºC and cooled down to 20 ºC in the magnetic field of H = 50 kA/m was from 121 to 182 % higher than magnetization of the as-sintered sample.

P.S.II.10.

Frequency behaviour of Co-based amorphous wire MI-element

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This study presents magnetoimpedance (MI) effect of Co-based amorphous wire investigated at driving frequency range $f \in$ [50 Hz – 5 MHz]. The XRD pattern and EDX analysis confirmed amorphous structure and the main element content of CoFeSiB alloy. The critical frequency of about 7 kHz was observed as the point with the initial increase of magnetoimpedance. A maximum MI-ratio $[Z(0) - Z(H_{\max})] / Z(H_{\max})$ of 334 % is attained at driving frequency of 900 kHz @ $H_{\max} \approx 4.63$ kA/m.

P.S.II.11.

Luminescence response of YAP: Mn crystal to the ionizing and visible radiation

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Optically stimulated luminescence (OSL) is used last decades as novel method of passive luminescence dosimetry and an alternative to the traditional thermo-luminescence dosimetry. One of the promising material for this application is crystalline $YAlO_3:Mn^{2+}$(YAP:Mn) [1]. But despite the similarity of physical processes during irradiation and stimulated luminescence OSL has a number of features. In particular, in contrast to thermo-luminescence, in which thermal activation of shallow traps makes them inactive when releasing deeper dosimetric traps, during optical stimulation released from the last charge carriers can be captured not only on deep traps but also on shallow ones, which leads to long afterglow. It was previously reported [2] that glow initiated by optical stimulation of irradiated YAP:Mn demonstrates the hyperbolic decay kinetics described by Becquerel's empirical law.

The present work is devoted to investigation of afterglow after X-ray irradiation as well as one induced by illumination by intense visible light produced by high power LEDs. The last is used in particular for the erasing of residual dosimetric signal optically.

Experiments have shown that the afterglow being registered up to 27 h could be produced by X-ray irradiation just for 10 s. Its initial level is saturating if the exposure time becomes more than 300 s. At the same time even illumination by red (660 nm) light can not only stimulate OSL but produce additional afterglow that should be taken into account in OSL dosimetric measurements based on YAP:Mn.

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P.S.II.12.

Activated Carbon Derived from Vine Shoots as Electrode Material for High-Performance Supercapacitors

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The wine industry produces large amounts of biomass waste, whose disposal and exploitation represents a problem for the environment. Most often, this waste is disposed of directly in the fields, which can cause a change in the composition of the soil and affect the life of plants. On the other side, biomass is the only alternative source of carbon from renewable sources. Activated carbon, thanks to its high electrochemical stability, large specific surface area, developed porosity and good electrical conductivity, is widely used in energy storage devices. That is why, in recent years, the development of biomass waste-to-energy valorisation technologies is a very active field of research. Here we present a simple method for obtaining low-cost and high surface area activated carbon (AC) from vine shoots. Synthesis includes carbonization of biomass precursor, which is followed by chemical activation at 700 °C. The prepared AC was characterized by FTIR spectroscopy and N_2 physisorption at -196 °C. FTIR spectra confirmed the changes in surface functionality of carbon after activation. N_2 adsorption/desorption studies revealed the presence of a highly developed system of micro- and mesopores in the activated sample, with a total specific area of 1494 m^2 g^{-1}. The supercapacitive performance and rate capability of the prepared AC were evaluated by Cyclic Voltammetry in aqueous electrolytes of different pH values (H_2SO_4, Na_2SO_4, KOH). The material has shown high stability in a wide range of scan rates and specific capacitance of ~163.4 F g^{-1} in H_2SO_4, ~142.4 F g^{-1} in Na_2SO_4 and ~171.3 F g^{-1} in KOH, at a scan rate of 20 mV s^{-1}. This research revealed that vine shoots can be considered new type biomass source to synthesize highly porous ACs for high-performance supercapacitors.

Acknowledgement: This work was supported by NATO Science for Peace and Security (SPS) Program (project G5836-SUPERCAR) and Ministry of Science of Montenegro (project BIOUGALJ).

P.S.II.13.

X-ray properties spectroscopy and electron structure of $Ca_3Ga_2Ge_4O_{14}$ garnet with dopped Ce (Eu)

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Crystals of $Ca_3Ga_2Ge_4O_{14}$ with the Ca-gallogermanate structure have a unique combination of physical properties - luminescent, laser, resilient, piezoelectric, and acoustic. Disordered trigonal compounds $Ca_3Ga_2Ge_4O_{14}$ activated with RE ions and transition elements are known as effective materials of quantum electronics, which combine the functions of generation and transformation of laser irradiation frequency. It stimulated the study of spectral - luminescent properties of transitional and RE metals impurity ions in these materials. However, the electronic structure, matrix luminescence of $Ca_3Ga_2Ge_4O_{14}$ crystals have not been sufficiently studied. The crystals were grown by Czochralski technique in the atmosphere of argon with adding oxygen using platinum crucible. The X-ray emission spectra of Ga (Ge) and Ce (Eu)L_{III}-edge in the $Ca_3Ga_2Ge_4O_{14}$garnet with dopped Ce 3 % and Eu 4% were obtained by a tube-spectrometer with X-ray coordinate detector of the original design. OKα-spectra in the $Ca_3Ga_2Ge_4O_{14}$garnet were obtained by a SARF -spectrometer. Spectra of the core levels and the valence band in the $Ca_3Ga_2Ge_4O_{14}$were measured by the “Kratos” X-ray photoelectron spectrometer. The X-ray spectral studies of the $Ca_3Ga_2Ge_4O_{14}$have shown that the top of the valence band (near the Fermi level) is formed mainly by the outer electron *p*–states of Ga, Ge, and O, which intensity is sufficiently low. The middle of the valence band is formed by the *Ga 3d*–states with the O*2s*–states lying below them. These states are hybridized with the 4*p*–states of Ga and Ge because of which they are $K\beta''$–satellite in $K\beta_2$– sub-band of *Ga* and *Ge*. The bottom of the valence band is formed by the 3*d*–states of germanium, which contribution in chemical binding is insignificant. Alignment of the X-ray emission bands of Ga and Ge with photoelectron spectrum of valence electrons of the $Ca_3Ga_2Ge_4O_{14}$demonstrated satisfactory correspondence.

P.S.II.14

Sol-gel based synthesis and magnetic, dielectric and optical properties study of nanocrystalline $Sr_3Co_2WO_9$ triple perovskite

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Perovskite materials have attracted extensive attention due to their fascinating properties and novel features attributed to the coexistence of ferro/ferri/antiferro-magnetic ground state and semiconductor band gap within the same material. In this research, triple perovskite $Sr_3Co_2WO_9$ has been successfully synthesized for the first time in the nanocrystalline form with an average crystallite size of 23 nm by means of a modified aqueous citrate sol-gel method. At room temperature, the crystal structure of $Sr_3Co_2WO_9$ is cubic, space group *Fm*-3*m* with lattice parameter a = 7.9073(6) Å. The formation of $Sr_3Co_2WO_9$ was studied *in situ* by X-ray diffraction and analysed by the Rietveld analysis. The detected hysteresis loops with non-zero remanent magnetization and rather large coercive field reveal ferrimagnetic ordering with Curie temperature of 144 K. The measured effective magnetic moment of $3\mu_B$ is close to the expected value for rarely observed intermediate spin $S = 1$. However, this can be also explained as a combination of LS (60 %) and HS (40 %) Co^{3+}. It is found that the compound exhibits the semiconducting properties with the optical band gaps equal to 3.52 eV (indirect) and 3.76 eV (direct), respectively. This was confirmed by AC conductivity measurements, which varies between 10^{-5} and 10^{-4} Ω^{-1} cm^{-1}. The Maxwell -Wagner model is employed to describe the frequency dependent dielectric constant. The frequency dependent AC conductivity follows the universal Jonscher’s power law. Semiconducting properties of this materials could thus be spin-controlled if implemented in devices.

P.S.II.15.

Sonochemical synthesis of up-converting β-$NaYF_4$: Yb, Er nanoparticles

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Up-converting nanoparticles (UCNPs) with unique ability to convert NIR to VIS light (anti-Stokes process) have a wide application in optoelectronics, forensic, security labeling and biomedicine. Over the past few years different methods (like co-precipitation, thermal decomposition, hydro/solvo thermal synthesis, *etc.*) are used for synthesis of β-$NaYF_4$: Yb/Er phase, mainly from toxic organic precursors. In this work we explore conditions for stabilization of β-$NaYF_4$: Yb/Er phase in nanoparticles applying sonochemistry synthesis of common inorganic precursor. The XRPD analysis showed that pure β phase is possible to obtained after 120 min of ultrasonification, while for shorter processing time (30-90min), cubic α-$NaYF_4$: Yb/Er or orthorhombic YF_3 : Yb,Er phase were founded too. The SEM and TEM analysis reveal presence of elongated nanoparticles self-assembled in spindles long up to 500 nm. Evolution of particle morphological and particle composition are analysed and correlated further with intensity of green emission ($^2H_{11/2}$,$^4S_{3/2}\rightarrow{}^4I_{15/2}$) intensity measured under excitation of 978 nm.

P.S.II.16.

Optoelectronic Processes through Molecular Nanofilms

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The model of the ultrathin (nano) film as spatially very confined (along one direction majorly narrowed) of molecular crystal structures is presented here. The theoretical analysis of the optoelectronic processes on all crystallographic planes and dielectric and optical properties of such samples was carried out using the Frenkel's exciton model and the Green's function method. The four-layered dielectric nanofilms with different boundary conditions on surfaces were researched and some discrete resonant absorption lines were obtained as a consequence of appearance of localized states in the surface layers. Their number and frequency position depend on the boundary parameter values. Unlike the corresponding balk-samples which are total absorbers throughout the near IR region, in ultrathin films will appear selective and discrete reflection and lager transparent region. These results can greatly contribute to optical nanoengineering, especially in the design of new photon equipment in nanomedicine to monitoring the movement of nanoparticles – drug carriers/deliverers.

P.S.II.17.

History and new trends in nanoSPD-related research

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In recent years, much attention in the scientific community as well as in industrial and business circles all over the world has been paid to nanostructured materials produced by severe plastic deformation (SPD) techniques, which generally, can be referred to as nanoSPD media, and this phenomenon only tends to progress with years. This is easily proven by publication activity within a vast number of international nano and, in particular, nanoSPD-related events held worldwide, even in present realia with many events taking place virtually or combining online and in-person presence.

In this report the scientometric approach is applied to analyse the data on research and developments in the nanoSPD field, *i.e.* the first pioneering works on a topic, methodology and technique as well as to trace the growing tendencies in modern research and applications. For this analysis, we use the most popular metrics, which are a journal's Impact Factor, number of citations for a publication and a researcher's h-index provided by such platforms as Web of Science Core Collection, Scopus, etc. In addition, with the help of emerging platforms, such as, for example, is a Brooklyn-based startup *scite* with the introduction of smart citations, we assess the publications with highest citations as supporting vs. disputing or neutral as they are cited in the text. Citation analysis is also used to establish and track the cutting-edge areas in research and thus predict whether or not the subject tends to grow and in what direction. Special attention in the report is focused practical application of bulk nanomaterials in engineering and medicine. The examples of successful use of nanostructured Ti alloys for the fabrication of medical implants of improved design and with increased functionality are demonstrated.

Acknowledgements: The research (for ZS) was in part supported by a grant of the Russian Science Foundation (project No. 19-49-02003).

P.S.II.18.

Anisotropic iron oxide nanostructures with potential applications in biomedicine

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Iron oxide based nanostructures have been developed during the last decade for magnetic data storage, sensors, specific cancer targeting, drug delivery and local physical effects (heat, radiation). We report nanochains (chain-like particles) consisted of silica-coated maghemite (γ-Fe_2O_3) nanoparticle clusters prepared by colloidal chemistry and magnetic field-induced self-assembly of nanoparticle clusters. The presented magnetic properties have revealed that the nanochains show a magnetic moment of the nanoparticles higher than the one of individual nanoparticle clusters. These differences can be attributed to the collective magnetic properties of superparamagnetic iron oxide nanoparticles (SPION) assembled in different morphologies, such as isotropic (spherical shape) and anisotropic (chain-like shape) morphology. We also find that is possible to achieve different magnetic properties with the nanochains depending only on their physical orientation.

P.S.II.19.

The influence of heteroatoms on physicochemical properties of cobalt ferrite nanoparticles

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In the last two decades, cobalt ferrite ($CoFe_2O_4$, CFO) has attracted extensive attention due to its applicability in data storage, catalysis, energy, environment, and in particular, biomedicine. To further extend applicability and improve understanding of fundamental processes, the present work investigates the influence of heteroatoms on physicochemical properties of CFO. Solvothermal method was used for designing a non-agglomerated particles with uniform morpho-structural properties. The physicochemical properties of Zn^{2+} and Ga^{3+} substituted CFO nanoparticles were examined ($Co_{(1-x)}Zn_xFe_2O_4$ and $CoGa_xFe_{(2-x)}O_4$; x=0, 0.1, 0.3 and 0.5). The X-ray diffraction (XRD) measurements confirmed the presence of pure cubic spinel phase in all samples, while the transmission electron microscopy (TEM) showed sphere-like nanoparticles with a mean diameter of 6±1 nm. The amount of adsorbed oleic acid on the surface of the nanoparticles, determined by thermogravimetric (TG) analysis indicates the formation of a complete monolayer of surfactant. The FT-IR analysis substantiated the presence of oleic acid on the surface of the nanoparticles and discovered its covalent bonding to the metal atoms. Substitution of host-atoms was also confirmed by Raman spectroscopy. Magnetic measurements revealed the influence of heteroatoms on saturation magnetization and magnetic anisotropy, showing for all the samples superparamagnetic behaviour at room temperature. The substitution of Co^{2+} and Fe^{3+} ions with Zn^{2+} and Ga^{3+}, respectively, leads to the change in chemical composition and cationic distribution of CFO and consequently to variation of its magnetic properties.

P.S.II.20.

Journey to the Center of a Perovskite Solar Cell

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Perovskite based solar cells have been one of the hottest topics in photovoltaic research as they have shown enormous potential for reaching high power conversion efficiency (PCE) in just a few years, going from only 3% just a decade ago to currently above 20 %. Coupled with the fact that the costs of the materials, synthesis and processing are very low, it is clear why these cells attract huge interest.
Recent studies suggest that porous structures can enhance device stability compared to planar structured devices. High synthesis temperatures and a limited selection of adequate materials are the main reasons why, although exhibiting record PCE for perovskite cells, alternatives to metal oxide based porous materials need to be studied. In this work, a novel organic-based interfacial layer was produced as cost efficient and scalable organics are the most promising alternatives to inorganic interfaces. With this novel layer, the perovskite effectively infiltrates into this mesoporous structure, and with enhanced wetting of the surface, the perovskite dramatically increases its homogeneity, thus leading to PCE enhancement and thermal stability. The characterized cell included a "n-i-p" architecture: Glass / ITO / SnO_2 / $PC_{61}BM$ / FAMAPbIBr / PDCBT / Ta-WO_X /Ag. Excluding the Ag electrode, the cell was processed entirely from solution by spin coating. Reported power conversion efficiency value was ~20 %.

P.S.III.1.

Thermodynamic Characteristics of Graphene

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The paper analyses the monolayer graphene and dispersion laws for phonons and electrons, and on the basis of these dispersion laws temperature dependences of the internal energy and specific heat of graphene are calculated. In dispersion laws for phonons, all three branches of acoustic phonons are included (while much lower contribution of three optical phonon branches is neglected). In dispersion laws for electrons, the cases of pure graphene and graphene with impurities and defects are considered (with calculated screened Coulomb interaction between the charge carriers in the second case). The temperature dependences of thermodynamic properties are given in graphical form and compared with the available experimental data.

P.S.III.2.

Ion beam irradiation of 12-tungstophosphoric acid – influence of energy of accelerated ions on structural properties

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Ion beam irradiation is a versatile tool for structural modification and engineering of new materials, where the energy of ions determines the nature of interactions between accelerated ions and the target. In this study, 12-tungstophosphoric acid (WPA) films of different thickness were spin-coated on platinized silicon substrate and irradiated with: low energy hydrogen ions (10 keV) and swift heavy ions (Bi, Xe and V) with energies up to 710 MeV. Raman spectroscopy and Fourier-transform infrared spectroscopy (ATR-FTIR) were used for investigation of structural properties of irradiated WPA. Raman spectra of irradiated samples revealed new wide vibrational bands in regions from 100 to 500 and 600 to 1000 cm^{-1} which are comparable to the ones obtained for WPA thermally treated at 600 °C. Additionally, bands of remaining Keggin anion structure appeared modified with observed shifting and splitting of bands. In ATR-FTIR spectra of irradiated samples additional wide bands at around 800 and 1100 cm^{-1} also appeared and resemble the ones of thermally treated WPA. The degree of change of these bands compared to the bands of Keggin anion was justified by SRIM calculations. The most prominent changes were observed in those samples for which the number of induced vacancies was the highest. The results show that structure of WPA can be tuned by ion beam irradiation, by optimizing the fluence and the type and energy of ions.

P.S.III.3.

Synthesis and deposition of $MAPbBr_3$ perovskite on titania nanotube arrays

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The organo-inorganic perovskites are materials that have recently revolutionized the field of photovoltaics due to their low-cost fabrication and high optical absorption. The hybrid organo-inorganic perovskite absorbs the visible part of the spectrum resulting in the creation of electron-hole pair. To decrease the recombination of charge carriers, the construction of solar cells requires the existence of separate layers for holes and for electrons. TiO_2 is usually used as an electron transport layer because its conduction band (CB) lies under the CB of perovskite. In that way, electrons diffuse from CB of perovskite to CB of TiO_2. For these experiments, TiO_2 nanotubular structure was used as an electron transport layer due to its advantages compared to nanoparticular TiO_2. TiO_2 nanotubes can provide a one-dimensional transmission channel for the charge carriers, so it will reduce the recombination rate of the carriers and provide a channel for fast carrier transport. However, there is a problem with the contact surface between perovskite and TiO_2 nanotubes. The aim of this study is to increase the contact surface of perovskite and TiO_2 nanotubes by filling the nanotubes with perovskite material in order to improve electron transport. Methylammonium lead bromide perovskite ($MAPbBr_3$) was deposited on anodically synthesized TiO_2 nanotubes which were annealed at 450 °C for 1 h. After degassation of the sample under high vacuum for 3 h at 200 °C, the cooled sample was put in a solution of $MAPbBr_3$ in dimethylformamide (DMF) and it was treated with inert gas (N_2), which enabled the filling of the nanotubes with perovskite material to some extent. FESEM and XRD analyses were used for morphological and chemical characterization of the sample. The diffuse reflectance spectroscopy measurement of the sample proved that deposition of $MAPbBr_3$ improves the absorption properties of TiO_2 nanotubes. By measuring the I-V characteristics of the sample in the dark and under visible light, a hysteresis curve was obtained.

P.S.III.4.

Application of biomass pyrolysis to obtain biofuels

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In this paper, the possibility of applying pyrolytic methods for obtaining biofuels from tobacco stems, as a residue after the process of its processing, was studied. The experiments of pyrolysis (which means heating the stem without the presence of oxygen), were performed at a temperature of 400 and 500 ^{o}C, in time periods of 30 and 60 minutes. Liquid pyrolysis products were analysed in detail using gas chromatographic mass spectrometry (GC-MS) techniques. The possibility of using the pyrolysis residue as biofuels, but also as an adsorption agent in the process of water remediation contaminated with organic and inorganic pollutants was studied. On the other hand, based on the results of the analysis of the obtained oils, the possibility of their application as fuels, but also as raw materials for obtaining various pharmacological products was assessed.

P.S.III.5.

Solubility of hydrogen in biomass-derived compounds relevant for hydrodeoxygenation process

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The production of many chemicals and materials is highly dependent on fossil fuels. Because of limited reserves and well-known disadvantages of using such energy sources, it is necessary to find appropriate renewable substitutes. Biomass has shown to be worthy of attention since it can be converted to biofuels and value-added chemicals relatively easily via hydrodeoxygenation (HDO) process. HDO involves reactions on solid catalyst in liquid solvent at high temperature and under hydrogen pressure. Therefore, the development of accurate kinetic models for HDO requires the knowledge on hydrogen solubility in biomass-derived compounds under various conditions.[1]

Dissolution of hydrogen in tetrahydrofuran (THF), furfuryl alcohol (FA) and tetrahydrofurfuryl alcohol (THFA) was studied in wide ranges of temperature and pressure and correlated by using the Soave-Redlich-Kwong equation of state (Fig. 1). Hydrogen solubility in furan[2] and THF[3] is very similar. The addition of hydroxymethyl group to the solvent's molecule (FA and THFA) significantly decreases the amount of the dissolved hydrogen and this effect is stronger in the case of unsaturated FA (Fig. 1).

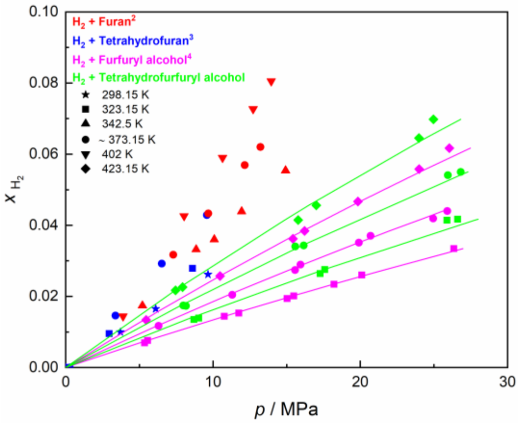

Figure 1. The comparison of hydrogen solubility in furan[2], THF[3], FA[4] and THFA. Lines represent the values calculated using SRK EoS with the optimized binary interaction parameters.

Acknowledgements: This work was funded by the Slovenian Research Agency (ARRS) under core funding P2-0152 and postdoctoral project Z2-9200

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P.S.III.6.

New environmentally acceptable materials based on flay ash, steelmaking slag and Zn-reach electric arc furnace dust

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The newer methods of electric arc furnace dust (EAFD) valorisation include its stabilization into materials which potentially can be used in construction. This is the most promising method because of the low costs and waste reduction. The purpose of these study was to investigate the properties of alkali activated cement (AAC) based on fly ash (FA) or steelmaking electric arc furnace slag (EAFS) as an agent fora stabilization/solidification of EAFD. The control type of AAC samples were prepared by mixing of solid precursor (FA or EAFS) with a mixture of 10 M NaOH and Na_2SiO_3 solutions followed by curing at in the oven for 48 h at 65 °C.

The samples of AAC doped with EAFD were prepared at the same conditions but the EAFD was added to the starting mixtures with FA in quantities of 10, 20 and 30% of total solid phase and 1, 2, 5 and 7 % of total EAFS solid phase.

The results have shown that both, FA and EAFS can be successfully used as an agent for EAFD stabilization. AAC samples based of FA and EAFS exhibited strength which is suitable for both, landfill and construction applications. Stabilization of EAFD into the AAC matrix occurred by chemical and physical immobilization. Chemical immobilization of Zn into the reaction product of FA and EAFS alkali activation was confirmed by SEM/EDS investigations.

The leaching of Zn from both, AAC matrix based on FA and EAFS is inferior in comparison to pristine EAFD and met the criteria for granular waste disposal at landfills for non-hazardous waste according the EN 12457-2 test.

P.S.III.7.

Effect of filler type on the physico-chemical and mechanical properties of metakaolin-based geopolymer composites

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Zircon ($ZrSiO_4$) is known to be a good refractory material, shows excellent chemical stability and resistance to thermal shock owing to the very low coefficient of thermal expansion and low coefficient of thermal conductivity. In addition, high purity sintered zircon retains its bending strength up to temperature as high as 1400 ^oC. These properties make zircon a promising structural ceramic for application where sudden temperature changes are expected. The high brittleness of geopolymers may be a limitation in some structural applications of geopolymers. To overcome this defect, a new class of geopolymer composites with addition of organic filler has recently been developed. In this research, geopolymer samples were synthesized by alkaline activation of metakaolin using a solution of NAOH molar concentration of 12M and the addition as inorganic filler Zircon 10, 20, 30 and 40 wt.% and as organic filler of 1 and 2 % PVA. The effect of zircon ($ZrSiO_4$) as inorganic filler and Poly-vinilalcohol as organic filler on the physico-chemical and mechanical.

P.S.III.8.

Synthesis and characterization of Schiff-base containing Metal-organic frameworks

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Metal-organic frameworks (MOFs) are promising efficient carbon-capture materials. One of the open challenges is their water sensitivity that either compete with carbon-dioxide or degrade MOF chemically. Our goal is to synthetize MOFs incorporating Schiff bases that will keep their carbon-dioxide adsorption capacity in presence of water, by chemically converting water into easily desorbing carbonyl compounds.
We investigated synthesis of Schiff base containing MOFs of different metal ions. MOFs containing free amine groups were prepared with two complementary strategies. Using 2-Aminoterephthalic acid and 2-Amino-[1,1'-biphenyl]-4,4'-dicarboxylic acid as bridging ligands in mild solvothermal conditions provided MOFs with amine groups covalently linked to the bridging ligands. Separately, amine groups were incorporated into UiO-67 type MOFs by a defect engineering strategy using an amine-containing monocarboxylate modulator. Both types of functionalized MOFs were post synthetically modified with selected carbonyl compound that can incorporate as an imine. Products are characterized by DTA, PXRD and FTIR spectroscopy.

This research was supported by the Science Fund of the Republic of Serbia, PROMIS, #6066708, CASCH-MOF; Erasmus+ KA1 between Keele University, United Kingdom and University of Novi Sad, Serbia.

P.S.III.9.

PVC Composites Reinforced by Metallurgical Waste from Ferro-Nickel Industry

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Industrial waste powders such as fly ash particles and slags are usually generated as an industrial by-product from the ferro-nickel production process and it is recognized as an environmental problem (hot spot). Due to the increased environmental concern, a significant effort on the FA utilization has been undertaken all over the world. One of the methods in circular economy and reuse of industrial waste is lowering the material cost is replacing components with not so expensive equivalents (mainly waste materials) but the substitution should be still accompanied by fulfilling the material and technical requirements. The main purpose of this work is use of solid waste materials from ferro-nickel industry (fly ash – FA, electric furnace slag – EFS and converter slag – CS) as a reinforcing component in polymer based composite – eco-friendly, functional geo-membranes.

The studied geo-membranes were produced by film-casting method using polyvinyl chloride (PVC) matrix reinforced by the previously mentioned metallurgical waste materials, as-prepared and modified in acid (HCl) and alkaline (NaOH) medium. The study of the produced geo-membranes was done related to their: i) morphology and internal structure (SEM observation and FTIR analysis), ii) thermal stability (TG/DTA/DTG analysis) and iii) moisture stability (followed kinetics of swelling was determined and the ultimate rate of swelling after 24 hours).

The morphology of the waste materials is of spherical and polygonal not regular shape and uniform. The morphology and microstructural properties of the obtained FA/PVC composites confirmed region of well dispersed particles where the particles were tightly embedded and mechanically interlocked in the PVC matrix indicating strong interfacial interaction with the polymer matrix. The studied composites (geo-membranes) have shown good thermal stability with corresponding low weight losses during thermal measurements. Generally, all the studied composites have shown higher swelling degree than PVC, where the composited reinforced with FA have shown the best performances in adsorption test.

P.S.III.10.

Effect of temperature and relative humidity on NO_x reaction with $CaCO_3$: competition between nitrite/nitrate formation on filter sheets

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In the present study, the influence of temperature and relative humidity on the nitrate/nitrite formation on the filter sheets, coated with fine grounded calcium carbonate (GCC), was investigated. Filter sheets were previously developed for the purpose of NO_x mitigation from ambient air. As a filter substrate "over-recycled" cellulose fibers, too weak to be used in further recycling, were used. The substrate was coated with GCC and micro-nano-fibrillated cellulose (MNFC), which was used as a binder and humectant. In reaction of GCC with NO_x gas, in the presence of moisture, calcium nitrate ($Ca(NO_3)_2$) can be generated. Bearing in mind that $Ca(NO_3)_2$ is considered as a premium fertiliser, further use of the material after use would be possible. The sample sheets were exposed to artificial NO_x gas in the climate chamber under different temperature (T = 5 and 20 °C) and relative humidity (RH of 20, 40, 60 and 90 %). Before NO_2 gas release from the cylinder (at volumetric flow of q 25 m^3 h^{-1}) and subsequent filter exposure for 8 h, all the pin coated sheet samples were conditioned for 10 h in the climate chamber on the set T and RH. The results reveal an increase in yield of $Ca(NO_3)_2$ on samples with an increase in RH, while nitrite at higher temperature (higher absolute humidity for same RH) does not convert to nitrate. In order to find out the practical effect of NO_x capturing by filter sheets, in addition, the samples were exposed to the higher concentration by using euro 5 diesel engine exhaust, under RH of 80 % and T = 60 °C for 80 min. with volumetric flow of q = 141.6 m^3 h^{-1} at flow rate of v = 3.57 m s^{-1}. The results after exposure to the „real" pollutant under different fluo-dynamic conditions reveal a higher yield of nitrate. It could be assumed that the higher pollutant flow over the sample's surface and specific way of applying GCC on the substrate by using the pin-coting method contribute to this. In addition, the NO_2 concentration after passing through the filter box (zig-zag folded filter papers longitudinally arranged by mesh carrier - to ensure over the surface filtration) is significantly reduced, by an average of 40 percent.

P.S.III.11.

Functionalization of polycaprolactone fibers by addition of yarrow extract powder

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There is a great potential to use polymeric fibres as drug carriers for biomedical applications, due to their possibility to deliver drugs at a controlled rate over a period of time at the site of action. Medicinal plants, including *Achillea millefolium* (yarrow) have been used traditionally for various purposes including wound healing. The positive effect of medicinal plants is attributed to the presence of bioactive molecules, primarily polyphenols. In this study, polycaprolactone (PCL), as a biocompatible polymer was combined with a yarrow extract powder. Previous experiments showed that yarrow extract can stimulate cell proliferation and has antimicrobial, antioxidant, and anti-inflammatory properties. Fibres mats were fabricated from PCL solutions containing yarrow extract powder at three concentrations (5, 10 and 15 % relative to the weight of the polymer) by using blend electrospinning method. *In vitro* release of yarrow polyphenols from the electrospun PCL fibres was investigated over a period of five days and showed release up to 98 % of the total loaded polyphenols. The antibacterial effect of PCL/yarrow electrospun fibres was examined against pathogen *Pseudomonas aeruginosa*. Yarrow extract retained its biological activity during the fabrication process and through incorporation into PCL fibres and could inhibit growth and biofilm formation of the tested pathogen. Based on the obtained results, yarrow loaded PLC fibres are multi-functional biomaterial that could prevent biofilm formation and presumably facilitate improved wound healing, which makes them suitable for production of catheter-coating materials or patches.

Acknowledgement: This work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Contract No. 451-03-9/2021-14/200287 and 451-03-9/2021-14/200135).

P.S.III.12.

Citric acid, polyethylene glycol, and hydroxypropyl methylcellulose as modifiers of doped calcium phosphate cement properties

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Biomaterials based on hydroxyapatite (HAp), having a similar mineral structure to minerals in teeth, represent suitable materials for demineralized caries-affected dentin layering. This study aimed to synthesize calcium phosphate cement, doped with Sr, Cu, and Zn ions. Doped calcium phosphate powder was obtained by modified hydrothermal synthesis, calcinated at 1500 ºC, followed by hand milling in an agate mortar. Liquid components for cement mixing consisted of citric acid (CA), CA with polyethylene glycol (PEG), and CA with PEG and hydroxypropyl methylcellulose (HPMC). Characterization of materials was determined by X-ray diffraction analysis (XRD), scanning electron microscopy (SEM), and energy dispersive X-ray analysis (EDX). After mixing with liquid components, net setting time, flow, and compressive strength were determined. *In vitro* bioactivity was assessed on SEM, after 15 days in simulated body fluid (SBF). XRD on specimens of calcinated doped powder showed α-tricalcium phosphate (α-TCP) as the dominant phase. EDX analysis confirmed the presence of all dopants in the powder. Compared to cement made with standard liquid (Na_2HPO_4), liquid with CA significantly decreased net setting time, followed by a slight increase with the incorporation of each additional liquid component. Flow of material decreased with the addition of citric acid and slightly increased with the addition of PEG, and PEG and HPMC. Compressive strength, after 15 days in SBF, regardless of the liquid components incorporated, showed satisfying values for dental luting materials. Cement with all experimental liquids showed *in vitro* bioactivity on the surface of the material, while when all three liquid components were included, the formation of Hap was observed on the cross-section as well. Bioactivity, mechanical properties, time of setting and handling properties of obtained cement based on α-TCP doped with Sr, Cu, and Zn ions, imply it could be further developed as a dental luting cement.

P.S.III.13.

Effect of Nb, Zr and Ta content on properties of Ti-Nb-Ta-Zr-O

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Titanium alloys belong to the perspective biomaterials used for orthopaedic implants, such as joint endoprostheses. The mostly studied alloying systems are composed of non-toxic beta stabilizing Nb and Ta. These elements enable the alloys to retain pure bcc beta phase after quenching from the beta region. The metastable beta phase can be tuned to have lower Young’s modulus which is crucial to avoid the stress shielding effect causing osteoporosis. In contrast, such alloys often suffer from low strength what limits their use. This shortcoming was reduced by adding a high content of oxygen (>0.5 wt%).

Several alloys with 0.7 wt.% of oxygen and different Nb, Ta and Zr content were designed and fabricated. Microstructure and phase composition were studied by means of scanning electron microscopy. Mechanical properties at room temperature were determined by microhardness measurements and tensile testing. Multiple compositions showing low Young’s modulus were found, while maintaining sufficient strength and ductility.

P.S.III.14.

3D printed mucoadhesive gelatin based buccal films

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The oral mucoadhesive film is a novel and attractive formulation for local and/or systemic drug delivery through the mucosal membrane of the oral cavity. Certain active pharmaceutical ingredients (API) in conventional formulations (tablets, capsules, syrups) are absorbed in the gastrointestinal tract and undergo first-pass metabolism through the liver, thereby reducing their bioavailability. This problem can be overcome by using intraoral formulations, such as mucoadhesive buccal films that disintegrate and dissolve in the oral cavity where the absorption of API occurs. In this work, the mucoadhesive films were prepared by 3D paste printing and the influence of processing parameters on film properties and the release rate of a drug was investigated. Gelatin (GA) and the blend of gelatin/polyvinylpyrrolidone (GA/PVP) were used because of their biocompatibility. Propranolol hydrochloride (PRH) was used as a model substance because it has high first-pass metabolism and is soluble in water. Film morphology and drug distribution were followed by SEM analysis. Dissolution test in simulated saliva was done to see how PRH was released from films. Mucoadhesion test revealed that the GA/PVP films with PRH have the highest adhesion force. Obtained results introduce GA/PVP as a promising material with good adhesion and rate of drug release.

Acknowledgement: This work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Contract No. 451-03-9/2021-14/200135 and No. 451-03-9/2021-14/200161)

P.S.III.15.

Improvement of bioactivity, biocompatibility, and antibacterial properties of titanium scaffold by coating with bioactive glasses and Ag-doped HAP

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Tissue engineering strategies for a treatment of large bone defects, which is currently implantation of bone grafts, are based on the development of biomaterials that mimic the bone tissue and improve regeneration. 3D printed macroporous titanium-based scaffolds, designed specifically for large bone defect implantation, provide both good mechanical support and architecture of pores suitable for ingrowth of bone tissue and better osseointegration. However, the bioinert surface of Ti6Al4V alloy is not the finest substrate for the growth of cells and mineral matrix deposition.

The aim of this study was to modify the surface of the macroporous Ti scaffold, by coating it with multiple layers of bioceramics: silicate bioactive glasses (BAG) and Ag-doped calcium hydroxyapatite (AgHAP), in order to provide bioactivity, biocompatibility, and antibacterial properties. A dip-coating technique was optimized to provide a thin coating that is homogenous and uniform inside the porous structure of titanium samples, followed by its melting at optimized temperature to acquire a continuous BAG layer covered with AgHAP particles.

The characterization of the synthesized bioceramic powders and surface morphology of specimen were conducted using scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy. The bioactivity was evaluated as the growth of hydroxyapatite crystals on the surface of the samples after 14 days in Simulated body fluid (SBF), which was determined using SEM. Biocompatibility of the obtained coatings and bare Ti samples was analyzed *in vitro* on the L929 cell line, applying the MTT test. Finally, the antibacterial properties of coated scaffolds were evaluated on *E.coli*, *S. aureus,* and *C. albicans*.

Evaluation of the morphology of the coatings showed that the homogenous deposition was achieved by a dip-coating method. Improved bioactivity, biocompatibility, and antimicrobial properties of the coated scaffold showed the great potential of this approach for future clinical application.

P.S.III.16

Modelling of catalytic activity and enzyme-MOF interactions using combined in silico approach

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Enzymes as industrial biocatalysts offer numerous advantages over traditional chemical processes concerning sustainability and process efficiency. Immobilization of enzymes on solid supporters is one of the key strategies for improving the practical performances of enzymes.
Metal-organic frameworks (MOFs) are promising candidates for enzyme immobilization. MOFs are porous coordination polymers consisting of metal-containing nodes and organic ligands linked through coordination bonds. It has been demonstrated that proteins can be successfully immobilized even in MOF pores whose apertures are smaller than the molecular dimension of the protein due to its conformational flexibility.
For our study, we selected horseradish peroxidase (HRP) encapsulated in MOF PCN-888(Al). We report the modelling of PCN-888(Al) MOF and the design of novel HRP mutants, which determine their enzymatic activity and magnitude of intermolecular interactions with MOF. Using a combined in silico approach, consisting of Informational Spectrum Method (ISM) bioinformatics method, molecular docking and molecular dynamics simulations, we propose new HRP mutants, which show higher/lower specific catalytic activity and higher/lower MOF-HRP dissociation constant, compared to the wild type of enzyme.

Acknowledgement: The work was funded by the Science Fund of the Republic of Serbia (Program PROMIS, project SYMBIOSIS, #6066997).

P.S.III.17.

Synthesis and characterization of Zn(II) and Bi(III) complexes with N-substituted glycine hydrazones

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The (*E*)-1-(2-oxo-2-(2-(quinolin-2-ylmethylene)hydrazinyl)ethyl)pyridin-1-ium chloride ligand, $\mathbf{HL^1}$Cl, was obtained from the condensation reaction of 2-quinolinecarboxaldehyde and Girard's P reagent in ethanol. Reaction of the ligand $\mathbf{HL^1}$Cl with $Zn(BF_4)_2 \cdot 6H_2O$ and NH_4SCN in molar ratio 1 : 1 : 2 in methanol/acetonitrile/water mixture resulted in formation of the mononuclear thiocyanato Zn(II) complex (**1**) with composition $[Zn\mathbf{L^1}(NCS)_2]$. The (*E*)-*N*,*N*,*N*-trimethyl-2-oxo-2-(2-(1-(thiazol-2-yl)ethylidene)hydrazinyl)ethan-1-aminium chloride ligand, $\mathbf{HL^2}$Cl, was obtained from the condensation reaction of 2-acetylthiazole and Girard's T reagent in water. Reaction of the ligand $\mathbf{HL^2}$Cl with $BiCl_3$ in molar ratio 1 : 1 in methanol/acetonitrile mixture resulted in formation of the mononuclear Bi(III) complex (**2**) with composition $[Bi\mathbf{HL^2}Cl_4]\cdot CH_3OH$.

The $[Zn\mathbf{L^1}(NCS)_2]$ complex has distorted square-pyramidal geometry, according to the X-ray, elemental analysis, NMR and IR spectroscopy. The tridentate hydrazone ligand is coordinated in deprotonated form to the Zn(II) with a NNO set of donor atoms and the other two coordination sites are occupied by thiocyanate ligands.

The X-ray crystal structure of complex **2** showed that Bi(III) ion has pentagonal-bipyramidal geometry. Bi(III) is coordinated with thiazole nitrogen, azomethine nitrogen and carbonyl oxygen atoms from non-deprotonated ligand and four monodentate chloro ligands. Furthermore, for characterization the elemental analysis and IR spectroscopy have been performed. However, due to the instability of the complex **2** in DMSO solution, NMR data are not available.

P.S.III.18.

Promising Hydroxyapatite/Nifuroksazid Conjugate

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The synergistic effect of two materials is a desirable phenomenon when designing a conjugate material. Synthetic Hydroxyapatite (HAp, $Ca_{10}(PO_4)_6(OH)_2$) is very similar to the inorganic part of bones and teeth of mammals. It is a well-known biomaterial with good biocompatibility, osteoconductivity and bioactivity. Nifuroxazide (NFX, $C_{12}H_9N_3O_5$) is a broad-spectrum antibacterial drug and poorly soluble in water. Nano HAp and NFX were mixed and homogenized in rotovapor giving as a result HAp/NFX conjugate. All materials were analyzed by Fourier transform infrared spectroscopy (FTIR), Field emission scanning electron microscopy (FESEM), X-Ray diffraction (XRD), Thermogravimetry (TG) and Brunauer–Emmett–Teller (BET) method. The *in vitro* antibacterial activities of HAp, NFX and HAp/NFX were examined against Gram-positive bacteria *Staphylococcus aureus*, Gram-negative bacteria *Escherichia coli* and yeast *Candida albicans*. *In vitro* drug release in simulated stomach acid and intestinal fluid showed a much faster release of NFX from HAp surface than those of raw drug. Afore mentioned analyses showed the unique properties of the HAp/NFX conjugate and introduced it as particularly prominent drug carrier.

Acknowledgements: This work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Contract No. 451-03-68/2021-14/200287 and 451-03-68/2021-14/200135).

P.S.III.19.

New biomaterials with saccharide components

III. The influence of trehaloses on cell membrane enzyme activity and some application in vaccine production

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Interest for supramolecular polymer systems (SUPLS) has grown highly last years, both in fundamental and application areas. Nowadays the investigations are induced also by the pandemic problems, but the synergetic cooperation and developments of polymer science, microbiology, molecular biology, and biophysical chemistry in that direction, were proposed already by Linus Pauling, exactly 70 years ago. Interestingly, the incentive in both periods, the one of early ideas emerging, and nowadays fast development, are related to virus issues, and vaccines, but the promising results extend to much broader areas: nano-technology and materials science, biology and bio-medicine, bio-engineering and pharmacy. Trehalose (TRH) was discovered in 1832 but Berthelot (who was than the leading person in both catalysis and biochemistry) was the one who isolated it from trehala (the product of wheat plants),gave it the name , and no wonder soon after, were discovered enzymes dealing with TRH in yeast cells. But the interest for it and its derivate *e.g.* trehalose 6-phosphate (TH-6P) decreased till 1970s when was discovered that yeast (YST) makes TRH under stress, to protect itself from desiccation and heat. But in spite many research efforts, and importance of water for environment and global heating issues, no explanation about the protective mechanism of THR is found. Some experiments indicate possible influences upon membrane ATPase functions, that is also vitally important and very complicated (SUPLS) system. In this contribution we consider possible interactions of TRH and TH-6P with P- ATPase, in particular protective role of TRH in either coating of the protein, (also in combination with polysaccharide pullulan, (PLU)), or binding TRH into its active site. Moreover, it is interesting because of opinion diversities, about actions of TRH-PLU materials, ranging from possibly of its use in vaccine production, till declaring it as high virulence factor. But the similar contraverses appeared with TH-6P, so Gussin declared it in 1972 as mystical “unicorn” - the legendary snark.

P.S.III.20.

Electrospun composite nanofibers containing biocompatible inorganic tungsten disulfide nanoparticles

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Tungsten disulfide nanoparticles (WS_2) emerged as excellent theranostics tool due to their exquisite optical properties and wide surface available for bioconjugation. However, their controlled delivery *in vivo* remains a challenge. Poly (lactic-co-glycolic acid) (PLGA) nanofibers are widely used as preferred carriers for the controlled release of drugs due to their biodegradability and their easy formation and preparation. In this study, the inorganic WS_2 nanoparticles demonstrated lack of cytotoxicity towards human peripheral blood mononuclear cells (PBMC) *in vitro* up to 100 µg/ml. Although these nanoparticles were easily internalized by monocytes, they did not modulate PHA-induced proliferation of PBMCs significantly. After loading of WS_2 with fluorescein isothiocyanate (FITC) as a model drug, they displayed similar cytotoxic profile in culture with PBMCs. PLGA composite nanofibers containing FITC-loaded WS_2 were prepared through an electrospinning solution technique. Field-emission scanning electron microscopy and *in-situ* scanning probe microscopy imaging were used to examine the morphology of the biocompatible nanoparticles and electrospun nanofibers, respectively. The distribution of fluorescent nanoparticles in the composite nanofibers was evaluated by fluorescence microscopy. Cumulatively, the electrospun composite nanofibers incorporated with biocompatible WS_2 inorganic nanoparticles represent new attractive theranostics platform, enabling a well-controlled delivery of bioactive molecules.

Acknowledgement: This work was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Contract No. 451-03-9/2021-14/200135) and by the Science Fund of the Republic of Serbia, PROMIS, #6062673, Nano-MDSC-Thera.

V.P.S.1.

Virtual Offline Poster Presentation

Cobalt based lamellar polymeric coordinated like-compounds as supercapacitors: linker effect on the enhancement of the charge capacity

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Recently, research focused on the use of energy storage devices have been increased as source of renewable energy. Thus, supercapacitors are a promising alternative, because of their high-power density. In this context, lamellar polymeric-coordinated structures have attracted great research interest due to their extraordinary properties such as fascinating construction. Two Co based lamellar polymeric like compounds were synthesized under vacuum and temperature with different linkers, water and pyrazine (Co-W and Co-P), which act as pillars between the layers formed by Co and terephthalic acid. Physicochemical characterization was carried out by XRD, FTIR, thermal analysis. Electrochemical studies were carried out at room temperature in a Multichannel potentio-stat−galvanostat, classic three-electrode cell, a graphite rod and Hg/HgO (1M NaOH) electrode as counter and reference electrode, respectively. The working electrodes were prepared by mixing Co-X materials, amorphous carbon, PTFE binder and ethanol onto stainless steel grids. From XRD and infrared results was confirmed the presence of lamellar structure, showing typical peaks and bands associated to the polymeric coordinated framework. Electrochemical techniques, Cyclic voltammetry (CV), Electrochemical techniques as EIS, SPECS and Galvanostatic Charge-Discharge curves (GCD) were employed to examine electrochemical and energy storage properties. The formation of two redox processes was observed for both materials, producing higher currents when pyrazine is present. It could be attributed to Co^{2+}/Co^{3+} redox pair with two different cobalt sites due to the dissimilar coordination of cobalt ion to the ligand, the processes are associated to diffusional a non-diffusional control effect. Energy storage processes are detected in the potential window, indicating the insertion and extraction of species from solution. From charge and discharge curves of electrodes at different current densities for Co-W and Co-P electrodes, the results exhibited that for all current densities, Co-P showed the larger capacity: 80 Cg^{-1}.

V.P.S.2.

Virtual Offline Poster Presentation

Multi-shelled Nickel oxide hollow-microspheres as bifunctional material for Electrochromic smart window and Non-enzymatic glucose sensor

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Nickel oxide (NiO) has been considered as one of the most promising candidates among various transition metal oxides due to its natural abundance, excellent electrochemical performances and obviously due to its environmentally benign nature. It has been observed that the morphology of a material plays a crucial role to upgrade its overall electrochemical properties, improving the kinetics of ion/electron exchange reactions. In this work, we obtained a facile hydrothermal route for the synthesis of NiO multi-shelled hollow microspheres. Here, carbonaceous saccharide microspheres had been used as sacrificial template to the formation of multi shells of NiO hollow microspheres. The multi-shells of the hollow spheres provide enhanced active surface area and additional reactive sites, which facilitate the faster ion intercalation and deintercalation, play key role in glucose sensing and electrochromism. This study offers a promising route to design advanced electrode materials for electrochromic smart windows and non-enzymatic glucose sensors.

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V.P.S.3.

Virtual Offline Poster Presentation

Investigation of (10%Co+0.5%Pd)/TiO_2(Al_2O_3) catalysts in the process of CO hydrogenation at low and high pressure

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Co-Pd catalysts are active in CO hydrogenation in synthesis gas. Many factors affect their activity and selectivity. Investigations at low and high pressure deliver information about the reasons and ways of product distribution. Properties of prepared in H_2 (10 % Co + 0.5 % Pd) / TiO_2(Al_2O_3) systems and their selectivity were studied by activity measurements, *in situ* DRIFTS, chemisorption of H_2 and CO, TPD and PCCS. Data obtained at 1 atm showed: WGSR proceeding; (Co-Pd)/TiO_2 samples were more active but (Co-Pd)/Al_2O_3 had higher selectivity to CH_4. Metal dispersion was very low due to pretreatment, reduction and agglomeration. (Co-Pd)/Al_2O_3 showed bimodal metal particles distribution, trend to easier agglomeration and facilitated alloying. CO adsorption was realized on highly varied sites. High temperature H_2 desorption from (Co-Pd)/Al_2O_3 determined presence of centers, which lead to increased number of species transferred to stronger adsorption sites for carbonate(-like) species on the support. CO species were firmly detained on the surface favouring hydrogenation both to CH_x and COH intermediates. (Co-Pd)/TiO_2 appeared SMSI even after contact with H_2O and air. Reaction was accompanied by surface reconstruction. Increase of T_{reac} concerned at higher extent increase of steadily adsorbed CH_x intermediate as revealed by DRIFTS study. The results testified that both systems had potential to produce C_{2+} hydrocarbons even at 1 atm. At 10.2 atm CO conversion and selectivity depended on T_{red}. CO conversion decreased with time. Compared to catalytic performance at 1 atm synthesis of C_{2+} hydrocarbons appeared and CO_2 amount decreased. CH_4 was the main product and CH_4/CO_2 ratio was higher for (Co-Pd)/Al_2O_3. CO conversion decrease is due to restricted diffusion from enhanced synthesis of C_{5+} hydrocarbons and metal particles agglomeration. Higher T_{red} favoured decrease in CO_2 production by WGSR due to higher extent of reduction, agglomeration and alloy formation.

Acknowledgement: The financial support of Bulgarian National Science Fund (КР-06-Н29-9) is appreciated.

V.P.S.4.

Virtual Offline Poster Presentation

Mechanical treatment of nitinol powder for hydrogenation by electrochemical methods

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Mechanical treatment of Ti-Ni powder with near-equiatomic composition was studied. The initial powder consists of mixture of phases TiNi (austenite) and (martensite), Ti_2Ni, $TiNi_3$ with the lattice parameters well correspond to literature data. After mechanical treatment of powders, the component with high width were appeared in the angle range from 40 to 48°, it corresponds to quasi-amorphous phase. It was established that the content of this phase increases up to 45 % after first ten seconds of treatment and does not significantly change for more milling time. The lattice parameter of all phases changes no more than 1 % after mechanical treatment. The widths of peaks significantly change after mechanical treatment more than 10 seconds, it could be connected with decrease of the coherently diffracting domain size due to an increase a dislocation density. The dislocation density was formed an estimate of using X-ray spectra and it was shown that these values reached up 10^{13} cm^{-2} which is a good agree with literature data. The average particle size measured by methods LD and BET decrease after mechanical treatment and corresponds to 0.5 and 2 μm at 300 seconds treatment respectively. The coherently diffracting domain size of TiNi (austenite) phase decreases from 26 nm to 4 nm with increasing of mechanical treatment time. The average particle size measured by SEM changes not monotonous with increasing of mechanical treatment time due to fracture and agglomeration of particles. It has been shown that only Ti_2Ni lattice parameter is significantly increase from $1.1315 \pm 3 \cdot 10^{-4}$ nm to $1.1617 \pm 3 \cdot 10^{-4}$ nm after hydrogenation that corresponds to formation the hydrides $Ti_2NiH_{0.5}$ and $Ti_2NiH_{0.8}$. Composition of hydride depends to hydrogenation time and mechanical treatment times.

Acknowledgement: This study was funded by RFBR, project number 19-38-90196.

V.P.S.5.

Virtual Offline Poster Presentation

Maximizing the Utilization of Active Species *via* Atomic Layer Deposition on Mesoporous Transition Metal Carbides: Next-Generation Electrodes for Highly Efficient OER Catalysis

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The production of green hydrogen from large-scale water electrolysers powered by renewable energy sources is an emerging technology to cut global carbon emissions and ease the depletion of fossil fuels.[1–2] In both electrolysers and fuel cells, platinum group metals (PGM) are typically employed as electrocatalysts. The oxygen evolution reaction (OER) is considered the main bottleneck for efficient electrochemical water splitting, as it requires high PGM catalyst loadings, e. g. based on scarce iridium.[3]

Transition metal carbides are promising materials for electrocatalytic reactions due to their excellent electrical properties.[4] However, a wide-spread application as a support material is hampered by an insufficient corrosion resistance under oxidative potentials in OER regime, which lead to undesired bulk oxidation, concomitantly decreasing electrical conductivity and, as a direct consequence, catalytic activity.

We present an innovative approach for the rational design of next-generation electrode coatings with the aim of maximizing the utilization of the catalytically active species for both acidic and alkaline OER. *Via* conformal atomic layer deposition (ALD) on high surface area transition metal carbides with template-controlled pore structure, well-controlled surface modifications with both PGM and non-precious metals were achieved. The catalysts show outstanding mass-specific activities and outperform literature-reported systems and commercial references by at least one order of magnitude at moderate overpotentials.

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V.P.S.6.

Virtual Offline Poster Presentation

Biomaterial based on nanostructured titanium with bioactive coating and its ability to the accelerated osteosynthesis

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The increase of human life expectancy and the progress in modern surgery require the development of the new generation metallic biomaterials with enhanced engraftment (improved bioactive properties). Clinical statistics show that the problem of implant’s rejection is relevant even for the latest models of implants.

The work is aimed at developing an integrated approach to produce a biomaterial capable of rapid osteosynthesis. The approach is based on a combination of bulk nanostructuring of the titanium matrix that improves its mechanical properties and surface nanostructuring by creating bioactive coatings that improves the properties of biomedical implants

In our work the approach is developed for the fabrication of a bioactive coating on titanium supports based on the modeling of the oxide films structure on nano- and microlevel. Developed textured bioactive coating allows to adjust the surface topography with high precision (down to 1 nm). This does not leads to the degradation of mechanical characteristics of titanium. Note also the high adhesion of the produced coatings to the titanium surface.

To obtain nano-coatings with controlled topography and surface structure, we use the chemical assembly method. The main advantage of this method is the possibility to produce nanostructures (nanocoatings) with high precision (down to Angstrom). Given that metal implants require the creation the strongly profiled surface at the nanoscale, the chemical assembly method is promising for the synthesis of bioactive nano-coatings.

Biomedical studies demonstrate that the resulting biomaterial has not only high adhesion surface for the investigated cell lines osteoblasts MS3T3-E1. Also, along with the adhesion, the initial cell differentiation of osteoblasts is observed. This phenomenon indicates the ability of this surface to the accelerated osteosynthesis.

Developed biomaterial can be used to obtain implants of new generation used in dentistry, reconstructive surgery and orthopedics.

Acknowledgments. This work was also supported in part by a grant from the St-Petersburg state university, No. id: 74883303

V.P.S.7.

Virtual Offline Poster Presentation

Nanostructured Cobalt@Polypyrrole and Cobalt/Gold@Polypyrrole materials: synthesis, optical and structural properties

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Nanocomposite materials based on conductive polymers and metal nanoparticles made an appearance as a new class of hybrid materials with considerable potential for application in different fields, from medical and food/wastewater treatments to catalysis and sensors. Besides their low cost and ease of preparation, their optical and mechanical characteristics are tunable, while individual features of each component become more obvious, and new ones appear. In this group of materials, newly, chemically synthesized Cobalt@Polypyrrole (Co@PPy) and Cobalt/Gold@Polypyrrole (Co/Au@PPy) nanocomposites could be classified. With low electrode potential, Co nanoparticles (CoNPs) are unstable, prone to oxidation and agglomeration. For this reason, both nanocomposites were synthesized under argon. Firstly, CoNPs were synthesized in water, by simple reduction of Co^{2+} by sodium borohydride and in the presence of sodium dodecyl sulfate as a surfactant that will stabilize formed Co nuclei and affect their further growth. After adding pyrrole monomer, the polymerization reaction was initiated by ammonium peroxydisulfate and Au^{3+} for Co@PPy and Co/Au@PPy, respectively. Together with pyrrole monomer oxidation to final polymer structure by Au^{3+}, these ions are reduced by nitrogen atoms from secondary amino groups in pyrrole units, forming AuNPs incorporated throughout polymer matrix. Conductive form of both nanocomposites, i.e., the presence of bipolarons, was confirmed by UV-Vis and FTIR analysis, while FESEM showed granular morphologies. With both nanocomposites having satisfactory percentage of metals incorporated, it could be expected that such materials could find their place in the field of catalysis, direct borohydride fuel cell, or wastewater treatment, where heavy, toxic metals such As(III) is, represent a great danger for the environment.

Acknowledgement: The research was funded by the Ministry of Education, Science and Technological Development of the Republic of Serbia, via direct financing of Vinča Institute of Nuclear Sciences – National Institute of Republic of Serbia (contract number: 451–03–68/2020–14/200017).

V.P.S.8.

Virtual Offline Poster Presentation

Creep behavior and microstructural changes of Inconel 625 nickel-based superalloy additively manufactured by L-DED method

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The aim of this work was to characterize the high temperature creep properties and evolution of the microstructure of 3D printed Inconel 625, manufactured by laser-assisted Direct Energy Deposition (L-DED) method. The as-built samples were subjected to stress relief annealing for 1 hour at a temperature of 870 °C. The microstructure was characterized by the cellular-dendritic substructure with numerous precipitates at the cell walls. Creep tests were conducted at a temperature of 600, 700 and 800 °C under a constant uniaxial tensile stress of 100 MPa according to ISO 204:2018 standard. The tests at 600 and 700 °C were performed for 2000 h, while at 800 °C the test was conducted until rupture after 700 h. The microstructure of creep-tested samples was investigated using scanning (SEM) and transmission electron microscopy (TEM).

Although, during the creep test at 600 °C the high tensile stress was applied, after the incubation time of 250 h, the shrinking of the sample occurred. A similar effect was recognized in the literature as a negative creep. Microstructural analysis has shown that this phenomenon was associated with precipitation of the γ'' (Ni_3Nb) particles, densely arranged inside the cells. A similar effect was revealed during the test at 700 °C after 100 h incubation time. In turn, after 2000 h of the test, the steady-state of creep deformation was achieved, which was associated with the microstructural changes consisting of the disappearance of the cellular substructure, extensive precipitation of plate-like precipitates of the δ phase at the prior cell walls, and formation of the network of carbides and Laves phase precipitates at the grain boundaries. The creep test at a temperature of 800 °C revealed relatively low creep resistance of L-DED Inconel 625. The sample was ruptured after 700 h while achieving 27% of the creep deformation. It was related to the intensification of the δ phase coarsening and the formation of cavities at the grain boundaries.

The results have shown the creep behavior of the L-DED Inconel 625 is strongly influenced by the evolution of precipitates, depending on the temperature and time of exposure.

This research was funded by AGH, Poland, grant no 16.16.110.663 - task 15 and the National Science Centre, Poland, grant no 2017/27/B/ST8/02244.

V.P.S.9.

Virtual Offline Poster Presentation

Swelling and deswelling kinetics of Au-PNiPAAm hydrogel nanocomposite photoactuators obtained by gamma irradiation

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In recent years, photoactuators as a class of smart materials that can produce a reversible mechanical deformation under light stimuli have attracted tremendous interest due to their potential applications in soft robotics, artificial muscles, and smart devices. Currently, the fabrication of photoactuators is mainly based on photothermal actuation mechanisms which include expansion/contraction, molecule sorption/desorption, and phase transition. Thermosensitive hydrogels with gold nanoparticles (AuNPs) are probably the most commonly used active layers that absorb light energy and convert it to thermal energy, causing reversible mechanical deformation such as bending, curling, and spiraling.

This work describes hydrogel nanocomposite photoactuators based on AuNPs and thermosensitive poly(N-isopropylacrylamide) (Au-PNiPAAm), obtained by gamma irradiation. The different shapes of AuNPs were incorporated into PNiPAAm hydrogel, nanospheres with radius ≈ 5-10 nm and nanorods with aspect ratio ~ 5 (radius ≈ 10 nm, length ≈ 50 nm). Swelling and deswelling kinetics of Au-PNiPAAm hydrogel nanocomposite photoactuators were investigated in water at 25°C and 48°C, respectively. All samples showed non-Fickian diffusion (both diffusion and polymer chains relaxation processes control the fluid transport) indicating that incorporation of different shapes of AuNPs into matrices has no influence on the diffusion model. On the other hand, the volume phase transition temperature (VPTT) of photoactuators can be adjusted by the incorporation of different shapes of AuNPs. It has been observed that VPTT decreases from ≈ 32.5°C for Au nanorods to ≈ 30.5°C for Au nanospheres, causing a more pronounced photothermal effect in the case of nanospheres.

Acknowledgements: This work was supported by the IAEA (CRP F22070, Contract No. 23184) and Ministry of Education, Science and Technological Development of the Republic of Serbia (Contract No. 451-03-68/2020-14/200017).

V.P.S.10.

Virtual Offline Poster Presentation

Zeolite/titania nanocomposites for photocatalytic degradation of dyes

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Nowadays, coloured effluents have become one of the major environmental issues because organic dyes and their degradation products are proven to have highly hazardous impact on human health and aquatic ecosystem. TiO_2 based photocatalysis have showed great potential for elimination of different contaminants. Main disadvantages of TiO_2 nanoparticles such as high tendency to agglomerate and expensive recovery process for further use can be prevailed by depositing TiO_2 on high surface area supports such as zeolites. The aim of this study was to develop zeolite/titania nanocomposites using facile and low-cost approach for efficient dye removal under simulated solar irradiation. Zeolite/titania nanocomposites were prepared by mixing different volumes of TiO_2 colloidal nanoparticles solution with selected zeolites (natural clinoptilolite (Cli) and synthetic ZSM-5). After 24 h of mixing, the nanocomposites were separated from solution by centrifuge and dried overnight. The physicochemical properties of nanocomposites were characterised by X-ray powder diffraction, UV-Vis diffuse reflectance (DR) spectroscopy, Fourier transform infrared spectroscopy (FTIR) and scanning electron microscopy with energy-dispersive spectroscopy (SEM-EDS). The parameters influencing photocatalytic process were also investigated (pH, reusability study, kinetics). Acid orange 7 (AO7) and acid red 18 (AR18) dyes were chosen for photodegradation tests as they are widely used in industry.

The loadings of TiO_2 colloidal nanoparticles obtained by EDS analysis were about 6 and 2 wt.% for nanocomposites based on Cli and ZSM-5 zeolite, respectively. Optical properties of TiO_2 nanoparticles were preserved according to UV-Vis DRS analysis. In spite of low amount of TiO_2 nanoparticles loaded onto the zeolite, the nanocomposites achieved complete discoloration of dyes aqueous solutions (AO7 and AR18) after only 40 minutes of irradiation. These findings suggest that using a simple, inexpensive preparation procedure efficient nanocomposites can be obtained.

V.P.S.11.

Virtual Offline Poster Presentation

g-C_3N_4/ZrO_2 nanocomposites: synthesis and application in photocatalysis

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In the quest to find suitable replacement for TiO_2 as omnipotent photocatalyst, but responsive in visible part of the spectra, graphitic carbon-nitride (g-C_3N_4) emerged. This metal-free indirect band-gap semiconductor, with band potentials at ~ -1.3 eV (CB) and ~ +1.4 eV (VB) (*vs.* NHE) and band-gap energy of approximately 2.7 eV, well suited in visible part of the spectra, is obvious candidate for water splitting reactions and/or formation of reactive oxygen species that are working force in photocatalytic degradation of pollutants. As such, it sounds as perfect photocatalyst, but there is a twist: it suffers from very fast recombination of photogenerated charges.

One of the ways to overcome this flaw is to make composites with other suitable semiconductor. In this study, we present our attempt to improve g-C_3N_4 by making its composites with ZrO_2, material with a conveniently positioned CB, at approximately -1.0 eV (vs. NHE) which could provide easily accessible „run-away“ point for g-C_3N_4 photogenerated electrons, leaving holes in its VB free to do the magic, and induce degradation of desired organic pollutants.

Potentials of VB and CB of composites, and pure components are determined by Mott-Schottky analysis, while optical characteristics of synthesized samples are obtained by DRS and PL spectroscopy. FTIR spectra are used to study structure of g-C_3N_4 and its composites.

Finally, the best composite with proven g-C_3N_4 - ZrO_2 bond, is probed in photocatalytic degradation of 2,4,6 - trichlorophenol under simulated solar light irradiation, and its performance is compared with pure g- C_3N_4.

Acknowledgement: Project of the Serbian Ministry of Education, Science and Technological Development, Grant no. 451-03-9/2021-14/200017 and Grant no. 451-03-68/2021-14/200026

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ACKNOWLEDGEMENTS

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ISBN 978-86-919111-6-4
9 788691 911164 >