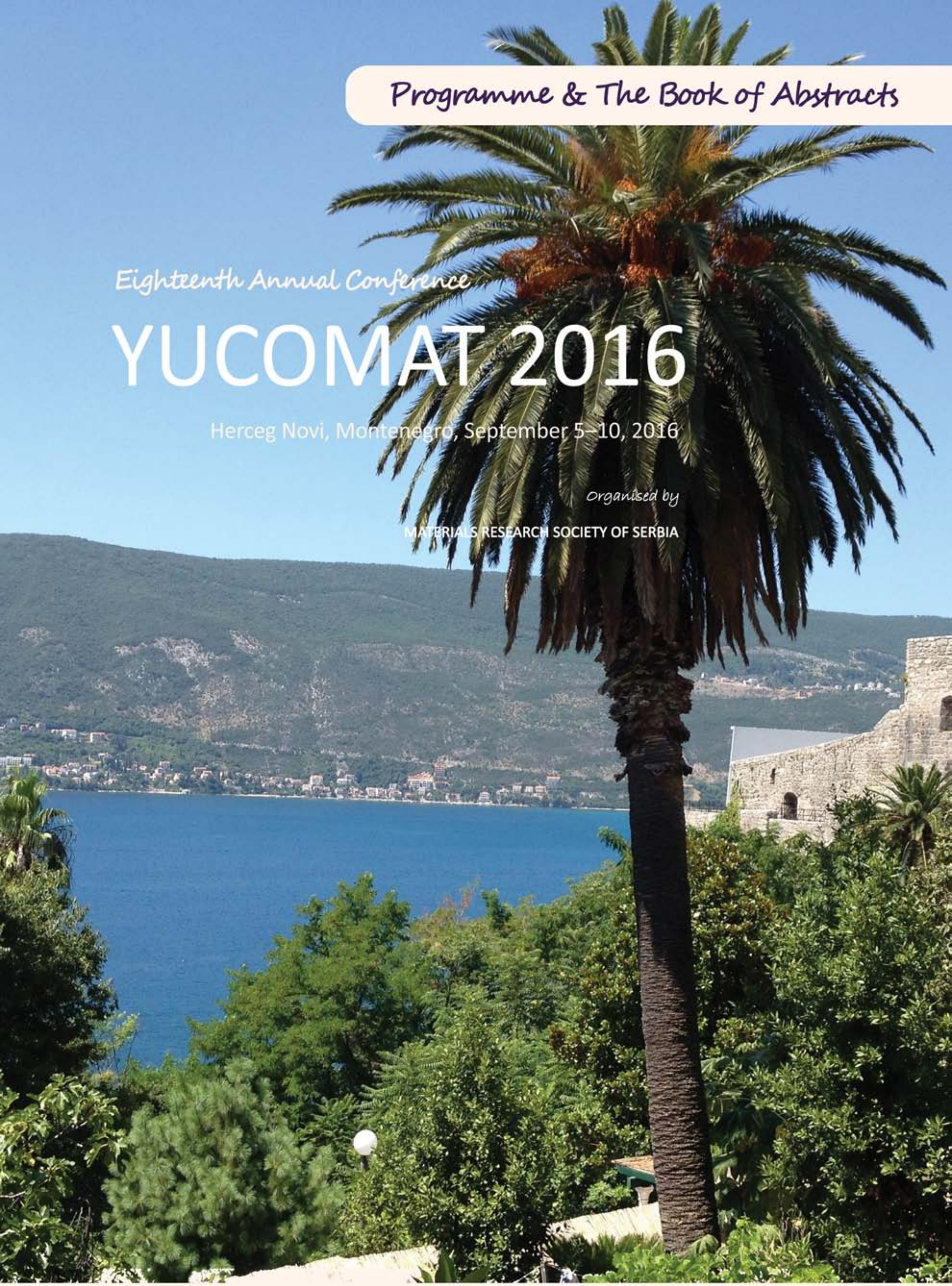

Programme & The Book of Abstracts

Eighteenth Annual Conference

# YUCOMAT 2016

Herceg Novi, Montenegro, September 5–10, 2016

Organised by

MATERIALS RESEARCH SOCIETY OF SERBIA

endorsed by

MRS E-MRS FEMS

## EIGHTEENTH ANNUAL CONFERENCE

# YUCOMAT 2016

Hunguest Hotel Sun Resort Herceg Novi, Montenegro,
September 5-10, 2016
http://www.mrs-serbia.org.rs

# Programme
# and
# The Book of Abstracts

Organised by:
**Materials Research Society of Serbia**

Endorsed by:
**Materials Research Society,**
**European Materials Research Society**
and
**Federation of European Material Societies**

**Title:** THE EIGHTEENTH ANNUAL CONFERENCE
**YUCOMAT 2016**
Programme and The 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; Fax: + 381 11 2185-263
http://www.mrs-serbia.org.rs

**Editors:** Prof. Dr. Dragan P. Uskoković and Prof. Dr. Velimir Radmilović

**Technical editor:** Aleksandra Stojičić

**Cover page:** Aleksandra Stojičić and Milica Ševkušić
Front cover: Modified photo by Boby Graham; Flickr
(https://www.flickr.com/photos/libertylittlebasil/7642177774/); CC BY-NC-SA 2.0
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**Acknowledgments:** This conference is held in honour of Prof. Dejan Raković's 65th birthday.

**Printed in:** Biro Konto
Sutorina bb, Igalo – Herceg Novi, Montenegro
Phones: +382-31-670123, 670025, E-mail: bkonto@t-com.me
Circulation: 220 copies. The end of printing: August 2016

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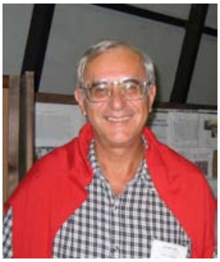
## WELCOME SPEECH BY THE PRESIDENT OF MRS-SERBIA:

**D**ear Participants of Eighteenth YUCOMAT,



**W**e have entered the third decade of our activities at YUCOMAT conferences, with no loss of enthusiasm, pace or quality. Quite contrary – if you were to ask me, I would tell you that we find ourselves on an upward slope; the quality of you, the participants of this year's meeting is in many respects higher than ever before. In spite of a plethora of small and big scientific conferences on materials science and engineering sprouting like mushrooms all across the globe, often in more prolific hubs for collaboration and connection with the advanced high-tech centers, we are disobeying the oft-foretold grim expectations and continue to deliver the best that the world has to offer in this field of science to the local scientific populace. YUCOMAT is now a well-recognized brand, so to speak, epitomizing a small meeting that is like wine produced in small batches, enjoyed only by the truest aficionados of conferences in the field of materials science and engineering and beyond.

**T**his year, the number of invited lecturers, all tremendous experts in their respective fields of materials science, is higher than ever before. Moreover, this year we have a large number of invited speakers who are joining us for the first time. It is difficult to assess which is the better indicator of our success at YUCOMAT: the fact that we traditionally have many recurrent speakers, who join us year after year, or the fact that there is a continuous interest among the newcomers, who hear positive things about the conference and express their interest to participate. You will find around 130 abstracts in the Book of Abstracts, describing the topics of talks and posters that will be presented this year by participants who have flown here from 34 different countries and practically all the continents of the world. Most of the participants are from Serbia (40), than from USA (13), Korea and Russia (11), Poland (10), Japan (7) and Germany (6). Contravening our intentions, however, the number of oral presentations and posters has not been on the increase throughout the past couple of years. Paradoxically, the least number of oral and poster presenters comes from the countries that the majority of the members of our International Advisory Board and of invited lecturers are affiliated with. Therefore, we expect that the faithful YUCOMAT "fans" will do more on its promotion and the attraction of younger participants from their institutions and the nearby centers in the years to come.

**A**s of last year, we have introduced the annual award for the lasting and exceptional contribution to materials science and engineering. This year's recipient of the award is Gordana Vunjak-Novakovic for her work in the field of Materials for Tissue Engineering and Regenerative Medicine (http://www.mrs-serbia.org.rs/index.php/award/2016-mrs-serbia-award-for-a-lasting-and-outstanding-contribution-to-materials-science-and-engineering). We are extraordinarily glad and honored to have her with us today. As a part of the Opening Ceremony, she will introduce you to some of her most significant research accomplishments.

**E**ver since the inception of YUCOMAT, we have made it an imperative to inspire and motivate young researchers through rewarding the best oral and poster presenters and the best doctoral theses defended in the timespan between two successive conferences. The same practice was adopted at our complementary conferences for young researchers, traditionally held at the Serbian Academy of Sciences and Arts in Belgrade in December. As of this year, we have introduced the subsidization of these prospective young scientists' participation at EUROMAT Junior conferences as a reward and as a response to the cordial promotion of YUCOMAT at the recently held EUROMAT Junior 2016 conference in Lausanne.

**I**n every segment of life, sustenance is possible only when coupled to ceaseless innovation. Therefore, we tirelessly seek for new contents at YUCOMAT. This year, for example, we have a seminal presentation of a distant, but in many respects very close country to us: Korea. When I say “close”, I mean that there is a plenty of instructive things that a small country can learn from the fantastic progress that the Korean economy has made in the past half a century or so by basing itself on the research-application-innovation triangle and its connection with high-tech industry. To this very day, Korean example stands as an unassailable one when it comes to the benefits that the economy of a small country can reap through smart and copious investments in basic research. Many of the participants of this symposium on Korean research in the field of science and technology of hybrid materials have been regular participants of YUCOMAT. All of the Korean experts this year participate through the invitation by the director of the National Core Research Center for Hybrid Materials Solutions of Busan University, Prof. Kwang Ho Kim, the director of KIST Institute for the Transfer of Technologies, Prof. Kyung Ho Shin, and myself, the president of MRS-Serbia. We intend to continue with this model and extend it as of the next year to Korea's neighbors, e.g., Singapore, Taiwan, China, Australia and Japan, so as to instigate the exchange of ideas and constructive collaborations.

**A**nother element of our mission for the future is the expansion of the network of scientists originating from the region of former Yugoslavia through these meetings. To that end, we strive to revert the devastating effect of “brain drain” - which was recently estimated to have the highest rate in the world in exactly this region - into the beneficial one of “brain gain”. Indeed, a very large number of researchers who earned their basic or highest degrees locally are now working at prestigious research centers worldwide. If each one of them was a node and they were all somehow interconnected, it would result in a fantastic network spanning the entire globe, yielding a structure of an enormous potential in revitalizing a country in which science is treated by governments more as a recreation and an expense with no expected returns than as an investment with unforeseeably high returns for present and future generations. One example of how well this could be done comes from our colleagues Davor Pavuna and Laszlo Forro and the conferences titled From Solid State to Biophysics held in the nearby Croatian town of Cavtat in June, which they have successfully organized for almost two decades now. Our plan is to organize a special symposium in which our scientists from abroad could present their research in the context of highlighting the benefits that emigration brought to their science and also promoting the ways in which it could benefit the country of their origins. We are currently on a good way to set up a team which would undertake this effort.

**F**or many years now, YUCOMAT conferences have been endorsed by the MRS, E-MRS and FEMS. Perhaps the strongest ties exist between MRS-Serbia and FEMS, which is logical given that MRS-Serbia has been a member of this Federation for almost ten years now. We wish to further strengthen these ties and our mutual work on organizing conferences such as EUROMAT, YUCOMAT, EUROMAT Junior and the MRS-Serbia’s Young Researchers conference offers room for this to become a reality.

**R**egarding the sponsors, we have had many of them at previous YUCOMAT conferences, but for the first time this year we have a Diamond Sponsor: FEI. It is our great pleasure that one such company with a tradition in the design and the manufacturing of microscope technologies has graciously decided to sponsor our conference, having recognized its regional importance and the quality of participants that they could reach. It is our hope that other companies presented at YUCOMAT, be they focused on materials synthesis, powder processing, the design of processed parts of various equipment or equipment *per se*, will follow this example.

**I**n closing, it is a part of the well-established tradition to symbolically dedicate every conference to anniversaries of one of our eminent members. This one will be dedicated to the Vice-President of MRS-Serbia, Prof. Dejan Rakovic, who turns 65 this year. Dejan is a cofounder of MRS-Serbia and he participated in practically all YUCOMAT conferences, significantly contributing to their becoming what they are today, for which we are immensely grateful to him.

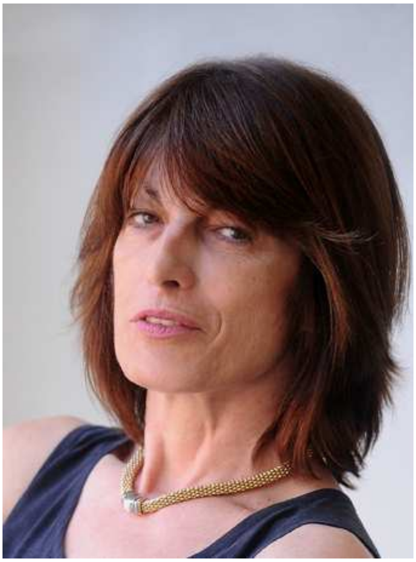
**S**incerely Yours,

**D**ragan Uskoković,

**P**resident of MRS-Serbia

## 2016 MRS-SERBIA AWARD FOR A LASTING AND OUTSTANDING CONTRIBUTION TO MATERIALS SCIENCE AND ENGINEERING

**W**e are pleased to announce that the recipient of the 2016 MRS-Serbia Award for a Lasting and Outstanding Contribution to Materials Science and Engineering is **Dr. Gordana Vunjak-Novaković** of Columbia University, New York, USA. She is awarded for her achievements in the field of Tissue Engineering and Regenerative Medicine.



**T**his is the decision of the MRS-Serbia Executive Board:

"**T**he Executive Board of the MRS-Serbia Presidency, on their meeting on March 15, 2016, considered submitted candidates for the MRS-Serbia's 2016 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, 2016, and that in the stipulated period of 45 days only one candidacy was submitted, that for Dr. Gordana Vunjak-Novaković, submitted by Prof. Dr. Milenko Plavšić. This submission was supported by: Prof. Dr Velimir Radmilović (Materials Science and Engineering) Belgrade University, Lawrence-Berkeley National Laboratory USA, corr. member of Serbian Academy of Sciences and Arts (SASA), Vice President of MRS-Serbia; Prof. Dr. Dejan Raković (Biophysics) Belgrade University, Vice President of MRS-Serbia; Prof. Dr. Nenad Ignjatović (Biomaterials) Institute of Technical Sciences of SASA, Academy of Engineering Sciences - Serbia; Prof. Dr. Stevo Najman (Cell Biology and Genetics) Medical School, University of Niš; Prof. Dr. Đorđije Šaranović (Medical Sciences) Medical School, Belgrade University, CCS; Prof. Dr. Gordana Ćirić Marjanović (Physical Chemistry of Polymers) Dean of The Faculty of Physical Chemistry, Belgrade University; Dr. Vukoman Jokanović (Biophysical Chemistry) Institute "Vinča" of Belgrade University, Engineering Academy of Serbia.

**H**aving received the opinion from the Expert Committee Members, Prof. Dr. Robert Sinclair, Prof. Dr. Danilo Suvorov and Dr. Ivan Božović, the Executive Board of the MRS-Serbia Presidency took the decision that Dr. Gordana Vunjak-Novaković be granted the MRS-Serbia's 2016 Award for a Lasting and Outstanding Contribution to Materials Science and Engineering.

**P**resident of MRS-Serbia, Prof. Dr. Dragan Uskokovic
**V**ice-President of MRS-Serbia, Dr. Slobodan Milonjić
**V**ice-President of MRS-Serbia, Prof. Dr. Velimir Radmilović
**V**ice-President of MRS-Serbia, Prof. Dr. Dejan Raković"

**D**r. Vunjak-Novaković's invited plenary lecture will be a part of the Opening Ceremony of the Eighteenth Materials Research Society of Serbia Annual Conference YUCOMAT 2016, which will be held in a beautiful little place at the Adriatic coast, Herceg Novi, Montenegro, September 5-10, 2016.

## MRS-Serbia

**President:** Dragan Uskoković
**Vice-presidents:** Slobodan Milonjić, Velimir Radmilović, Dejan Raković
**Members:** Snežana Bošković, Milorad Davidović, Vera Dondur, Nenad Ignjatović, Djuro Koruga, Nedeljko Krstajić, Slavko Mentus, Zoran Petrović, Milenko Plavšić, Zoran Popović, Vladimir Srdić, Momčilo Stevanović, Jovan Šetrajčić, Miodrag Zlatanović

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## Conference Organising Committee

**Chairperson**: Nenad Ignjatović
**Members**: Nikola Cvjetićanin, Ivana Jevremović, Dragana Jugović, Smilja Marković, Branko Matović, Jovan Mirković, Nebojša Mitrović, Željka Nikitović, Irena Nikolić, Bojana Obradović, Nebojša Romčević, Edin Suljovrujić, Milan Tadić, Đorđe Veljović, Mira Vukčević
**Conference Secretary:** Aleksandra Stojičić

## Conference Technical Committee

Ivana Jevremović, Vuk Radmilović, Vladimir Rajić, Zoran Stojanović, Milica Ševkušić

## HISTORY:

Materials science and engineering incorporate acquiring of knowledge on synthesis and processing of materials, their composition and structure, properties and behaviour, functions and potentialities as well as application of that knowledge to various final products. Economic prosperity, life quality, and healthy environment are tightly connected with the improvements in the existing and the development of new materials and processing technologies. These improvements and development can contribute greatly to the national priorities: energy saving, environment and health protection, information and communication, infrastructure, transportation, etc.

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).

## GENERAL INFORMATION

**DATE AND VENUE:** The conference will be held on September 5-10, 2016, at the Hunguest Hotel Sun Resort, in Herceg Novi, Montenegro. Participants will also be accommodated there. The conference will begin on Monday, September 5th, at 09.00 and end on Friday, September 9th, 2016, at 13.00.

**REGISTRATION:** Registration, registration fee payment, conference materials distribution, etc, will take place at the conference desk (Conference Secretariat) open on Sunday, September 4, Monday, September 5, and Tuesday, September 6, from 8.00 to 19.00, on 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.

**INSTRUCTION FOR AUTHORS:** The conference will feature plenary sessions, oral sessions, poster sessions, and an Exhibition of synthesis and characterization equipment.
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 registration, specifying the name of the speaker and the day and session number.
In POSTER SESSIONS, the authors are requested to display their posters minimum one hour before the session and to be present beside their posters during the session. Poster sessions' venue will be open from Tuesday to Thursday, from 18.00-22.00.

**CONFERENCE AWARDS:** Materials Research Society of Serbia will award the authors (preferable young members under 35) of the best oral and poster presentation at the conference, and also the authors of highly rated PhD theses defended between two conferences. Awarded researchers are granted free registration at the next YUCOMAT Conference.

**ADDITIONAL ACTIVITIES:** An Exhibition of synthesis and characterization equipment will be held during the Conference. Traditional Cocktail Party on Monday evening and excursions on Wednesday afternoon to Dubrovnik (Croatia), Thursday afternoon (boat trip around Boka Kotorska Bay) will be organized again. Full day excursion will be organized on Saturday, also.

# Programme

# GENERAL CONFERENCE PROGRAMME

**SYMPOSIUM A**: Advanced Methods in Synthesis and Processing of Materials
**SYMPOSIUM B**: Advanced Materials for High-Technology Application
**SYMPOSIUM C**: Nanostructured Materials
**SYMPOSIUM D**: Eco-materials and Eco-technologies
**SYMPOSIUM E**: Biomaterials
**SYMPOSIUM F**: Advanced hybrid and composite materials

*Sunday, September 4 2016*

| | |
|---|---|
| $08^{00}$-$19^{00}$ | **Registration** |

*Monday, September 5, 2016*

| | |
|---|---|
| $08^{00}$-$09^{00}$ | **Registration** |
| $09^{00}$ -$10^{00}$ | **OPENING CEREMONY**<br>- Introduction and Welcome<br>Main Conference Hall |
| $10^{15}$-$13^{15}$ | **First Plenary Session**, Main Conference Hall |
| $13^{15}$ | **Photo Session** |
| $15^{00}$-$19^{00}$ | **Symposium F**, Main Conference Hall |
| $19^{30}$-$21^{00}$ | **Cocktail Party** |

*Tuesday, September 6, 2016*

| | |
|---|---|
| $08^{30}$-$12^{30}$ | **Second Plenary Session**, Main Conference Hall |
| $15^{00}$-$16^{30}$ | **Symposium C**, Main Conference Hall |
| $17^{00}$-$19^{00}$ | **Symposium E**, Main Conference Hall |
| $15^{00}$-$16^{15}$ | **Symposium B**, Small Conference Hall |
| $16^{45}$-$17^{30}$ | **Symposium D**, Small Conference Hall |
| $20^{00}$-$22^{00}$ | **Poster Session I** (Symposium A), Villa Mimoza |

*Wednesday, September 7, 2016*

| | |
|---|---|
| $08^{30}$-$12^{30}$ | **Third Plenary Session**, Main Conference Hall |
| $14^{00}$-$19^{00}$ | **Excursion to Dubrovnik, Croatia** |
| $20^{00}$-$22^{00}$ | **Poster Session II** (Symposium B), Villa Mimoza |

*Thursday, September 8, 2016*

| | |
|---|---|
| $08^{30}$-$12^{30}$ | **Fourth Plenary Session**, Main Conference Hall |
| $14^{00}$-$19^{00}$ | **Boat-trip around Boka Kotorska Bay** |
| $20^{00}$-$22^{00}$ | **Poster Session III** (Symposiums C and E), Villa Mimoza |

*Friday, September 9, 2016*

| | |
|---|---|
| $09^{00}$-$12^{30}$ | **Fifth Plenary Session**, Main Conference Hall |
| $12^{30}$-$13^{00}$ | **Awards and Closing of the Conference** |

*Saturday, September10, 2016*

| | |
|---|---|
| Full day | **Excursion to Skadar, Albania"The last Secret of Europe"** |

## OPENING CEREMONY

*Monday, September 5, 2016*
**Main Conference Hall**

**$09^{00}$-$10^{00}$**

**Welcome Speach**
Dragan Uskoković, President of MRS-Serbia, Belgrade, Serbia
**Presentation of YUCOMAT 2015 Awards**
Slobodan Milonjić, Vice President of MRS-Serbia

**MRS-Serbia 2016 Award for a Lasting and Outstanding Contribution to Materials Science and Engineering**
**Cell-instructive biomaterials for tissue engineering: Applications in regenerative medicine and study of disease**
Gordana Vunjak-Novaković
Columbia University, Department of Biomedical Engineering, Laboratory for Stem Cells and Tissue Engineering, New York, NY, USA

**Break: $10^{00}$-$10^{15}$**

## FIRST PLENARY SESSION

**Main Conference Hall**

**Session I: $10^{15}$-$11^{45}$**
**Chairmen: Gordana Vunjak-Novakovic and Robert Sinclair**

$10^{15}$-$10^{45}$ **Stimuli-responsive smart soft materials**
Takuzo Aida
The University of Tokyo and RIKEN Center for Emergent Matter Science, Tokyo, Japan

$10^{45}$-$11^{15}$ **Therapeutic biomaterial devices for controlled drug release in ocular and cardiac disease treatment**
Freddy Boey, Subbu Venkatraman
Nanyang Technological University, School of Materials Science and Engineering, Singapore

$11^{15}$-$11^{45}$ **Iron oxide nanoparticles for medical application: still a challenging task**
Heinrich Hofmann
Powder Technology Laboratory, Institute of Materials, Ecole Polytechnique Federale de Lausanne, Switzerland

**Break: $11^{45}$-$12^{15}$**

**Session II: $12^{15}$-$13^{15}$**
**Chairmen: Takuzo Aida and Velimir R. Radmilović**

$12^{15}$-$12^{45}$ **In situ electron microscopy of energy-related thin film reactions**
Robert Sinclair, Sang Chul Lee and Ai Leen Koh
Department of Materials Science and Engineering and Stanford Nano Shared Facilities, Stanford University, CA, USA

$12^{45}$-$13^{15}$ **Lithium and scandium trialuminides embedded in solid matrix**
Velimir R. Radmilović
Serbian Academy of Sciences and Arts, Knez Mihailova 35, 11000, Beograd, Serbia

**$13^{15}$-$13^{45}$ Photo session**

**Break: $13^{45}$-$15^{00}$**

## SYMPOSIUM F: ADVANCED HYBRID AND COMPOSITE MATERIALS

**Main Conference Hall**

**Session I: $15^{00}$-$17^{00}$**
**Chairpersons: Kwang-Ho Kim, Robert Sinclair, Danilo Suvorov and Margarethe Hofmann**

$15^{00}$-$15^{30}$ **Materials research in Europe – a new concept needed?**
Margarethe Hofmann-Amtenbrink[1], Alessandra Hool[2]
[1]Past President of FEMS, CEO MatSearch and Foundation of Rare Metals, ESM, Pully, Swiss, [2]MatSearch and Foundation of Rare Metals, ESM, Pully, Swiss

$15^{30}$-$16^{00}$ **Hybrid-interface materials**
Kwang Ho Kim[1,2]
[1]Global Frontier R&D Center for Hybrid Interface Materials, Busan, Republic of Korea, [2]School of Materials Science and Engineering, Pusan National University, Busan, Republic of Korea

$16^{00}$-$16^{15}$ **Advanced nanotechnology based on the directed self-assembly of block copolymers for device applications**
Woon Ik Park, Jung-Ho Cho, Young Hun Jeong, and Jong Hee Whang
Electronic Materials & Component R&D Center, Korea Institute of Ceramic Engineering & Technology (KICET) 101 Soho-ro, Jinju 52851, Republic of Korea

$16^{15}$-$16^{30}$ **Virus based novel colorimetric sensor for cancer cell detection**
Suck Won Hong[1], Jin-Woo Oh[2]
[1]Department of Cogno-Mechatronics Engineering, Pusan National University, Busan 46241, Republic of Korea, [2]Department of Nanoenergy Engineering, Pusan National University, Busan 46241, Republic of Korea

$16^{30}$-$16^{45}$ **Organic-inorganic hybride thin films using atomic/molecular layer deposition for flexible electronic applications**
Jin-Seong Park
Division of Materials Science and Engineering, Hanyang University, Seoul, Republic of Korea

$16^{45}$-$17^{00}$ **Ultrathin ALD interfacial layer for improved materials properties**
Zhixin Wan, Woo-Jae Lee, Kwang-Ho Kim, and Se-Hun Kwon
School of Materials Science and Engineering, Pusan National University, Republic of Korea

**Break: $17^{00}$-$17^{30}$**

**Session II: $17^{30}$-$19^{00}$**
**Chairpersons: Kwang-Ho Kim, Robert Sinclair, Danilo Suvorov and Margarethe Hofmann**

$17^{30}$-$18^{00}$ **3-Dimensional hybrid nanostructures: Novel fabrication strategies and applications**
Yeon Sik Jung
KAIST- Korean Institute for Science and Technology, Seoul, Republic of Korea

$18^{00}$-$18^{15}$ **Hybrid materials/device enabling high energy and power densities along with robust cycle life**
Jeung Ku Kang, Hyung Mo Jeong, Il-Woo Ock, Jong Ho Weon
Department of Materials Science & Engineering and Graduate School of EEWS, Daejeon, Republic of Korea

$18^{15}$-$18^{30}$ **Multi-scale computational design of active and durable materials for renewable energy systems**
Byungchan Han, Joonhee Kang, Jeemin Hwang, Seunghyo Noh, Choa Kwon
Department of Chemical and Biomolecular Engineering, Yonsei University, Seoul, 03722, Republic of Korea

$18^{30}$-$18^{45}$ **$Ni_2Si$ silicide wire fabrication by conventional metal alloy processing**

Seung Zeon Han[1], Sung Hwan Lim[2], Byungchan Han[3] and Kwang Ho Kim[4]
[1]Commercialization Research Division, Korea Institute of Materials Science, Changwon, Republic of Korea, [2]Department of Advanced Materials Science & Engineering, Kangwon National University, Chuncheon, Republic of Korea, [3]Department of Chemical and Biomolecular Engineering, Yonsei University, Seoul, Republic of Korea, [4]School of Materials Science and Engineering, Pusan National University, Busan, Republic of Korea

$18^{45}$-$19^{00}$ **Developing multi-component coatings for structural applications by a hybrid HIPIMS technique**

Qimin Wang[1], Kwang Ho Kim[2]
[1]School of Electromechanical Engineering, Guangdong University of Technology, Guangzhou, P.R. China, [2]Global Frontier R&D Center for Hybrid Interface Materials, Pusan National University, Busan, Republic of Korea

# SECOND PLENARY SESSION

*Tuesday, September 6, 2016*
**Main Conference Hall**

**Session I: 08$^{30}$-10$^{30}$**
**Chairpersons: Eva Olsson and Hamish Fraser**

08$^{30}$-09$^{00}$ **In situ off-axis electron holography of two-dimensional transition metal dichalcogenides**
Rafal E. Dunin-Borkowski[1], Florian Winkler[1], Amir H. Tavabi[1], Juri Barthel[2], Martial Duchamp[1], Emrah Yucelen[3], Sven Borghardt[4], Beata E. Kardynal[4]
[1]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons and Peter Grünberg Institute 5, Forschungszentrum Jülich, D-52425 Jülich, Germany, [2]Gemeinschaftslabor für Elektronenmikroskopie (GFE), RWTH Aachen University, D-52074 Aachen, Germany, [3]Faculty of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, D-48047 Duisburg, Germany, [4]Peter Grünberg Institute 9, Forschungszentrum Jülich, D-52425 Jülich, Germany

09$^{00}$-09$^{30}$ **Real-time viewing of III-V semiconductor nanowire growth by In Situ TEM**
L. Reine Wallenberg[1], F. Lenrick[1], M. Ek[1], D. Jacobsson[1], L. Samuelson[2] and K. Dick Thelander[1]
[1]nCHREM, Inst. for Chemistry; [2]Solid State Physics, Lund University, Sweden

09$^{30}$-10$^{00}$ **Oxidation of carbon nanotubes using environmental TEM and the influence of the imaging electron beam**
Ai Leen Koh[1], Emily Gidcumb[2], Otto Zhou[2,3] and Robert Sinclair[4]
[1]Stanford Nano Shared Facilities, Stanford University, Stanford, CA 94305, USA, [2]Department of Applied Physical Sciences, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599, USA, [3]Department of Physics and Astronomy, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599, USA, [4]Department of Materials Science and Engineering, Stanford University, Stanford, CA 94305, USA

10$^{00}$-10$^{30}$ **Electric field and thermal induced effects in nanostructured materials revealed by advanced in situ electron microscopy**
Ludvig de Knoop, Hanna Nilsson, Andrew Yankovich, Norvik Voskanian, Lunjie Zeng and Eva Olsson
Department of Physics, Chalmers University of Technology, 412 96 Gothenburg, Sweden

**Break: 10$^{30}$-11$^{00}$**

**Session II: $11^{00}$-$12^{30}$**
**Chairmen: Rafal E. Dunin-Borkowski and Gianluigi A. Botton**

$11^{00}$-$11^{30}$ **Energy loss spectroscopy at high resolution: Applications to functional oxides and nanostructures**
Gianluigi A. Botton
McMaster University, Department of Materials Science and Engineering, 1280 Main Street West, Hamilton, Ontario, Canada

$11^{30}$-$12^{00}$ **Non-planar nanostructures at atomic scale**
Jordi Arbiol[1,2]
[1]Institució Catalana de Recerca i Estudis Avançats (ICREA), 08010 Barcelona, CAT, Spain, [2]Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and The Barcelona Institute of Science and Technology, Campus UAB, Bellaterra, 08193 Barcelona, CAT, Spain

$12^{00}$-$12^{30}$ **The art and science of spatially-resolved determinations of local composition in an aberration-corrected electron microscope**
Brian Welk, Jacob Jensen, John Sosa, Dan Huber, Robert Williams, Babu Viswanathan, and Hamish L Fraser
Center for the Accelerated Maturation of Materials, Department of Materials Science and Engineering, The Ohio State University, Columbus, OH, USA

**Break: $12^{30}$-$15^{00}$**

## SYMPOSIUM C: NANOSTRUCTURED MATERIALS

**Main Conference Hall**

**Session I: $15^{00}$-$16^{15}$**
**Chairpersons: Satoshi Ohara and Natalia Kamanina**

$15^{00}$-$15^{15}$ **Structural characterization of organic bulk heterojunction solar cells**
Vuk V. Radmilović[1], Fei Guo[2], Christoph J. Brabec[2,3], Erdmann Spiecker[4], Velimir R. Radmilović[5]
[1]Innovation Center, Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia, [2]Institute of Materials for Electronics and Energy Technology (i-MEET), Friedrich-Alexander-University Erlangen- Nuremberg, Erlangen, Germany, [3]Bavarian Center for Applied Energy Research (ZAE Bayern), Erlangen, Germany, [4]Center for Nanoanalysis and Electron Microscopy (CENEM), Friedrich – Alexander - University of Erlangen- Nuremberg, Erlangen, Germany, [5]Serbian Academy of Sciences and Arts, Belgrade, Serbia

$15^{15}$-$15^{30}$ **High-performance Ni-GDC nanocomposite anode fabricated from GDC nanocubes for low-temperature solid-oxide fuel cells**
Satoshi Ohara and Kazuhiro Yamamoto
Joining and Welding Research Institute, Osaka University, Japan

$15^{30}$-$15^{45}$ **The chemical recycling of polycarbonate using $CeO_2$ nanocatalysts**
Minori Taguchi, Takashi Naka, Toshitaka Funazukuri
Chuo University, National Institute for Materials Science, Tokyo, Japan

$15^{45}$-$16^{00}$ **Modification of the materials properties via surface structuring**
Natalia V. Kamanina
[1]Vavilov State Optical Institute, Kadetskaya Liniya V.O., dom.5, korpus 2, St.-Petersburg, 199053, Russia, [2]Saint-Petersburg Electrotechical University (“LETI”), St. Petersburg, Russia

$16^{00}$-$16^{15}$ **Half Heusler thermoelectics $Ti_{(1-x)}Fe_{(1.33+x)}Sb$ - TiCoSb**
Ali Tavassoli[1,2,3], A. Grytsiv[1,3,4], G. Rogl[1,3,4], V. Romaka[5], P. Broz[6,7], E. Bauer[3,4], G. Giester[8], M. Zehetbauer[2], P. Rogl[1,4]
[1]Institute of Materials Chemistry and Research, University of Vienna, Waehringerstr. 42, A-1090 Wien, Austria, [2]Faculty of Physics, University of Vienna, Boltzmanngasse 5, A-1090 Wien, Austria, [3]Institute of Solid State Physics, Vienna University of Technology, Wiedner Hauptstr., 8-10, A-1040 Wien, Austria, [4]Christian Doppler Laboratory for Thermoelectricity, Wien, Austria, [5]Department of Materials Science and Engineering, Lviv Polytechnic National University, Ukraine, [6]Masaryk University, Faculty of Science, Department of Chemistry, Kotlarska 2, 611 37, Brno, Czech Republic, [7]Masaryk University, Central European Institute of Technology, CEITEC, Kamenice 753/5, Brno 62500, Czech Republic, [8]Institute of Mineralogy and Crystallography, University of Vienna, Althanstraße 14, A-1090 Vienna, Austria

$16^{15}$-$16^{30}$ **Shape directing agents for controlling the morphology of anisotropic iron oxide nanoparticles**
Ana Mraković[1], Gurvinder Singh[2], Frode Seland[2], Erzsébet Illés[1], Nikola Knežević[1], Vladan Kusigerski[1], Sanja Vranješ-Đurić[1], Vojislav Spasojević[1] and Davide Peddis[1,3]
[1]The Vinča Institute of Nuclear Sciences, Belgrade, 11001, Serbia, [2]Department of Materials Science and Engineering, Norwegian University of Science and Technology, Trondheim-7491, Norway, [3]Istituto di Struttura della Materia – CNR, 00016 Monterotondo Stazione (Roma), Italy

**Break: $16^{30}$-$17^{00}$**

## SYMPOSIUM E: BIOMATERIALS

**Main Conference Hall**

**Session I: 17$^{00}$-19$^{00}$**
**Chairpersons: Nenad Ignjatović and Bojana Obradović**

17$^{00}$-17$^{15}$ **Multifunctional opto-magnetic NaYF$_4$:Er$_{3+}$,Yb$_{3+}$,Gd$_{3+}$&Fe$_3$O$_4$@SiO$_2$ nanoconstructs – towards biomedical applications**

Bożena Sikora[1], Przemysław Kowalik[1], Krzysztof Fronc[1], Jakub Mikulski[1], Izabela Kamińska[1], Anna Borodziuk[2], Magdalena Duda[2], Katarzyna Łysiak[3], Maciej Szewczyk[4,5], Karolina Zajdel[6], Grzegorz Gruzeł[7], Leandro C. Figueiredo[8], Paulo C. Morais[8,9], Laise Andrade[10], João P. Longo[10], Ricardo B. de Azevedo[10], Zulmira G. M. Lacava[10], Ewa Mosiniewicz-Szablewska[1], Magdalena Parlińska-Wojtan[7], Roman Minikayev[1], Tomasz Wojciechowski[1], Anita Gardias[3], Jarosław Rybusiński[3], Andrzej Sienkiewicz1[1,12], Mariusz Łapiński[13], Piotr Stępień[4,5,14], Wojciech Paszkowicz[1], Jacek Szczytko[3], Andrzej Twardowski[3], Małgorzata Frontczak-Baniewicz[6], Danek Elbaum[1]

[1]Institute of Physics, Polish Academy of Sciences, Warsaw, [2]Division of Biophysics, Institute of Experimental Physics UW, Warsaw, [3]Institute of Experimental Physics, Faculty of Physics UW, Warsaw, [4]Institute of Genetics and Biotechnology, Faculty of Biology UW, Warsaw, [5]Institute of Biochemistry and Biophysics PAS, Warsaw, [6]Mossakowski Medical Research Centre PAS, Warsaw, [7]Institute of Nuclear Physics PAS, Krakow, [8]Instituto de Fisica, Universidade de Brasilia, Brasilia DF, Brazil, [9]College of Chemistry and Chemical Engineering, Anhui University, Hefei, China, [10]Instituto de Ciências Biológicas, Departamento de Genética e Morfologia, Universidade de Brasilia, Brasilia DF, Brazil, [11]Laboratory of Physics of Complex Matter, EPFL, Station 3, Lausanne, Switzerland, [12]ADSresonaces, Préverenges, Switzerland, [13]Institute of Optoelectronics, Military University of Technology, Warsaw, [14]Centre of New Technologies, Ochota UW, Warsaw, Poland

17$^{15}$-17$^{30}$ **Tumor-selective hybrid system based on hydroxyapatite nanocarrier, chitosane, poly(lactic-co-glycolic acid) and androstan derivate**

Nenad L. Ignjatović[1], Katarina M. Penov-Gaši[2], Victoria M. Wu[3], Jovana J. Ajduković[4], Vesna V. Kojić[4], Dana Vasiljević-Radović[5], Vuk D. Uskoković[3,6], Dragan P. Uskoković[1]

[1]Institute of Technical Sciences of SASA, Belgrade, Serbia, [2]University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Novi Sad, Serbia, [3]Advanced Materials and Nanobiotechnology Laboratory, Department of Bioengineering, University of Illinois, Chicago, IL, USA, [4]Oncology Institute of Vojvodina, Sremska Kamenica, Serbia, [5]University of Belgrade, Institute for Chemistry, Technology and Metallurgy, Belgrade, Serbia, [6]Department of Biomedical and Pharmaceutical Sciences, School of Pharmacy, Chapman University, Irvine, CA, USA

$17^{30}$-$17^{45}$ **One pot and two step synthesis of 1D and 2D calcium phosphates and their biomedical characteristics**

Zoran S. Stojanović [1], Nenad Ignjatović [1], Victoria Wu [2], Vojka Žunič [3], Ljiljana Veselinović [1], Srečo Škapin [3], Miroslav Miljković [4], Vuk Uskoković [2,5], Dragan Uskoković [1]

[1]Institute of Technical Sciences of SASA, Knez Mihailova 35/4, 11000 Belgrade, Serbia, [2]Advanced Materials and Nanobiotechnology Laboratory, Department of Bioengineering, University of Illinois, 851 South Morgan Street, Chicago, IL 60607-7052, USA, [3]Advanced Materials Department, Jožef Stefan Institute, Jamova cesta 39, 1000 Ljubljana, Slovenia, [4]Laboratory for Electron Microscopy, Faculty of Medicine University of Niš, Dr. Zoran Đinđić Boulevard 81, 18 000 Niš, Serbia, [5]Department of Biomedical and Pharmaceutical Sciences, School of Pharmacy, Chapman University, 9401 Jeronimo Road, Irvine, CA 92618-1908, USA

$17^{45}$-$18^{00}$ **Alginate hydrogels with silver nanoparticles and honey as potential wound dressings**

Bojana Obradović[1], Jasmina Stojkovska[1], Vesna Mišković-Stanković[1], Milica Labudović Borović[2], Ljiljana Šćepanović[2]

[1]Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia
[2]School of Medicine, University of Belgrade, Belgrade, Serbia

$18^{00}$-$18^{15}$ **Novel platforms for designing antimicrobial biomaterials**

Marija Vukomanović, Vojka Žunič, Mario Kurtjak, Nemanja Aničić, Danilo Suvorov
Advanced Materials Department, Jozef Stefan Institute, Ljubljana, Slovenia

$18^{15}$-$18^{30}$ **Coupling vanadate elution control with catalytic properties of $V_2O_5$ in $V_2O_5$/PLGA composite coating**

Nemanja Aničić[1,2], Marija Vukomanović[1], Danilo Suvorov[1]

[1]Advanced Materials Department, Jožef Stefan Institute, Ljubljana, Slovenia
[2]Jožef Stefan International Postgraduate School, Ljubljana, Slovenia

$18^{30}$-$18^{45}$ **Quantifying the fractal dimension and the effective permeability of membrane fouling**

Miguel Herrera-Robledo and Volodymyr V. Tarabara
Department of Civil and Environmental Engineering, Michigan State University, USA

$18^{45}$-$19^{00}$ **Effect of cooling rate from $\alpha+\beta$ range on stereological parameters of microstructure in the $Ti_6Al_7Nb$ alloy**

Krzysztof Wieczerzak, Robert Dąbrowski, Edyta Rożniata, Rafał Dziurka
AGH University of Science and Technology, Faculty of Metals Engineering and Industrial Computer Science, Al. A. Mickiewicza 30, 30-059 Kraków, Poland

# SYMPOSIUM B: ADVANCED MATERIALS FOR HIGH-TECHNOLOGY APPLICATIONS

**Small Conference Hall**

**Session I: 15⁰⁰-16¹⁵**
**Chairmen: Zoran S. Petrović and Smilja Marković**

15⁰⁰-15¹⁵ **Boson peak and glass forming ability in CuHfTi metallic glasses**
Amra Salčinović Fetić[1,2], G. Remenyi[3,4], D. Starešinić[2], E. Babić[5], I. A. Figueroa[6], H. A. Davies[7], and K. Biljaković[2,3]
[1]Department of Physics, Faculty of Science, University of Sarajevo, Sarajevo, Bosnia and Herzegovina, [2]Institute of Physics, Zagreb, Croatia, [3]CNRS, Institut Néel, Grenoble, France, [4]Institut Néel, Université Grenoble Alpes, Grenoble, France, [5]Department of Physics, Faculty of Science, Zagreb, Croatia, [6]Institute for Materials Research-UNAM, Ciudad Universitaria Coyoacan, Mexico D.F., Mexico, [7]Department of Engineering Materials, University of Sheffield, Sheffield, UK

15¹⁵-15³⁰ **The influence of thermal treatment on physicochemical properties of graphene oxide/phosphotungstic acid nanocomposite**
Zoran Jovanović[1], Danica Bajuk-Bogdanović[2], Milica Vujković[2], Željko Mravik[2], Ivanka Holclajtner-Antunović[2]
[1]Laboratory of Physics, Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia, [2]Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia

15³⁰-15⁴⁵ **Influence of point defects concentration on optical and photocatalytic properties of ZnO ceramics**
Smilja Marković[1], Vladimir Rajić[2], Ljiljana Veselinović[1], Jelena Belošević-Čavor[3], Srečo Davor Škapin[4], Stevan Stojadinović[5], Vladislav Rac[6], Steva Lević[6], Miloš Mojović[2], Dragan Uskoković[1]
[1]Institute of Technical Sciences of SASA, Belgrade, Serbia, [2]Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia, [3]The Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia, [4]Jožef Stefan Institute, Ljubljana, Slovenia, [5]Faculty of Physics, University of Belgrade, Belgrade, Serbia, [6]Faculty of Agriculture, University of Belgrade, Zemun, Serbia

15⁴⁵-16⁰⁰ **Activated track etched carbon for supercapacitor electrodes**
Petar Laušević, Predrag Pejović, Dragana Žugić, Yuri Kochnev, Pavel Apel and Zoran Laušević
[1]Laboratory of physical chemistry, Vinča institute of nuclear sciences, University of Belgrade, Serbia, [2]School of Electrical Enginering, University of Belgrade, Serbia, [3]Flerov laboratory of nuclear reactions, Joint institute for nuclear research, Dubna, Russia

$16^{00}$-$16^{15}$ **The influence of fluorine doping on the structural and the electrical properties of $LiFePO_4$ powder**
Dragana Jugović[1], Miodrag Mitrić[2], Miloš Milović[1], Nikola Cvjetićanin[3], Bojan Jokić[4], Ana Umićević[2], Dragan Uskoković[1]
[1]Institute of Technical Sciences of SASA, Knez Mihailova 35/IV, 11 000 Belgrade, Serbia, [2]Vinča Institute of Nuclear Sciences, University of Belgrade, P.O. Box 522, 11 001 Belgrade, Serbia, [3]Faculty of Physical Chemistry, University of Belgrade, Studentski Trg 12-16, P.O. Box 137, Belgrade, Serbia, [4]Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11 000 Belgrade, Serbia

**Break: $16^{15}$-$16^{45}$**

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

**Small Conference Hall**

**Session I: $16^{45}$-$17^{30}$**
**Chairmen: Smilja Marković and Irena Nikolić**

$16^{45}$-$17^{00}$ **Designing materials from biological oils**
Zoran S. Petrović
Pittsburg State University, Kansas Polymer Research Center, USA

$17^{00}$-$17^{15}$ **Recovery of rare earth elements of bastnasite ores by advanced hydrometallurgical methods**
Carsten Dittrich[1], Srećko Stopić[2], Bernd Friedrich[2]
[1]MEAB Chemie Technik GmbH, Aachen, Germany
[2]IME Process Metallurgy and Metal Recycling, Germany

$17^{15}$-$17^{30}$ **Strength and durability of alkali activated slag in a sea water: influence of alkali ion**
Irena Nikolić[1], Smilja Marković[2], Ljiljana Karanović[3], Vuk Radmilović[4], Velimir Radmilović[5]
[1]University of Montenegro, Faculty of Metallurgy and Technology, Džordža Vašingtona bb, 81 000 Podgorica, Montenegro, [2]Institute of Technical Sciences of SASA, Knez Mihailova 35, Belgrade, Serbia, [3]University of Belgrade, Faculty of Mining and Geology, Laboratory of Crystallography, Đušina 7, 11000 Belgrade, Serbia, [4]Innovation center, University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11120 Belgrade, Serbia, [5]Serbian Academy of Sciences and Arts, Knez Mihailova 35, Belgrade, Serbia

# THIRD PLENARY SESSION

*Wednesday, September 7, 2016*
**Main Conference Hall**

**Session I: $08^{30}$-$10^{30}$**
**Chairmen: Eiji Osawa and Francois M. Peeters**

$08^{30}$-$09^{00}$ **Grain boundary geometry, structural units and segregation in oxides**
Yuichi Ikuhara[1,2,3]
[1]Institute of Engineering Innovation, The University of Tokyo, Tokyo, 113-8656, Japan, [2]Nanostructures Research Laboratory, Japan Fine Ceramics Center, Nagoya, 456-8587, Japan, [3]WPI-AIMR Research Center, Tohoku University, Sendai, 980-8577, Japan

$09^{00}$-$09^{30}$ **Interfacial step alignment as a mechanism of hetero-epitaxy/orientation relationships: the case of Ag on Ni**
Dominique Chatain[1], Paul Wynblatt[2], Anthony D. Rollett[2], Gregory S. Rohrer[2]
[1]Aix-Marseille University, CNRS, CINaM, UMR 7325, 13288 Marseille, France, [2]Department of Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, PA 15213, USA

$09^{30}$-$10^{00}$ **Controlling Microstructural Evolution via Adsorption**
Wayne D. Kaplan
Department of Materials Science and Engineering, Technion - Israel Institute of Technology, Israel

**Break: $10^{00}$-$10^{30}$**

**Session II: $10^{30}$-$12^{30}$**
**Chairpersons: Dominique Chatain and Yuichi Ikuhara**

$10^{30}$-$11^{00}$ **TEM observation of atomic structures and their evolutions in 2D and 1D materials**
Kazu Suenaga
Advanced Industrial Science and Technology, Ibaraki, Japan

$11^{00}$-$11^{30}$ **Atomic Structure of defects, dopants and edge terminations in monolayer 2D materials**
Jamie H. Warner
Department of Materials, University of Oxford, UK

$11^{30}$-$12^{00}$ **Atomic collapse in graphene**

Francois Peeters[1], Dean Moldovan[1], Massoud R. Masir[1,2], Eva Andrei[3]
[1]Department Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerpen, [2]Department of Physics, University of Texas at Austin, Austin TX 78712, USA, [3]Rutgers University, Department of Physics and Astronomy, Piscataway, NJ 08855, USA

$12^{00}$-$12^{30}$ **Aberration corrected views of of chemical ordering and segregation in complex oxides**

Maria Varela
Facultad de CC. Fisicas & Instituto Pluridisciplinar, Universidad Complutense de Madrid, 28040 Madrid, Spain

# FOURTH PLENARY SESSION

*Thursday, September 8, 2016*
**Main Conference Hall**

**Session I: $08^{30}$-$10^{30}$**
**Chairmen: Danilo Suvorov and Philippe Colomban**

$08^{30}$-$09^{00}$ **Towards device physics of the $CH_3NH_3PbI_3$ photovoltaic perovskite**
László Forró
Laboratory of Physics of Complex Matter, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausannes, Switzerland

$09^{00}$-$09^{30}$ **Tailoring defined-shape ferroelectric particles for various ferro- and piezoelectric applications**
Danilo Suvorov[1], M. Macek-Krzmanc[1] and H. Ursic Nemevsek[2]
[1]Advanced Materials Department, Jožef Stefan Institute, Jamova 39, Ljubljana, Slovenia, 1000, [2]Electronic ceramics Department, Jožef Stefan Institute, Jamova 39, Ljubljana, Slovenia, 1000

$09^{30}$-$10^{00}$ **How could electrolytes and electrodes be friendlier for Li-ion traffic?**
Mamoru Senna
Faculty of Science and Technology, Keio University, Japan

**Break: $10^{00}$-$10^{30}$**

**Session II: $10^{30}$-$12^{30}$**
**Chairmen: Mamoru Senna and László Forró**

$10^{30}$-$11^{00}$ **Recent progress in R&D of the primary particles of detonation nanodiamond**
Eiji Osawa, Shuichi Sasaki, Ryoko Yamanoi
NanoCarbon Research Institute Limited, Ueda, Japan

$11^{00}$-$11^{30}$ **Nanodiamond and its derivatives for catalysis**
Dangsheng Su
Dalian Institute of Chemical Physics, Chinese Academy of Science, Dalian, China

$11^{30}$-$12^{00}$ **Scaffolds for tissue repair and regeneration**
Serena Best
University of Cambridge, UK

$12^{00}$-$12^{30}$ **Advanced and in situ transmission electron microscopy of semiconductor nanowire materials**

Wolfgang Jäger
Institute of Materials Science, Christian-Albrechts-University of Kiel, 24143 Kiel, Germany, EU

## FIFTH PLENARY SESSION

*Friday, September 9, 2016*
**Main Conference Hall**

**Session I: $09^{00}$-$11^{00}$**
**Chairmen: Jamie H. Warner and Wolfgang Jäger**

$09^{00}$-$09^{30}$ **Neutron scattering and atomistic modeling for materials science**
Max Avdeev
Australian Nuclear Science and Technology Organisation, Lucas Heights, Australia

$09^{30}$-$10^{00}$ **Understanding failure and fatigue mechanisms of advanced and natural polymer fibres by Raman/IR microspectrometry**
Philippe Colomban
Sorbonne Universités, UPMC Paris 06, MONARIS umr8233 CNRS, France

$10^{00}$-$10^{30}$ **High-melting point compounds: new approaches and results**
Rostislav A. Andrievski
Institute of Problems of Chemical Physics, Semenov Prospect, 1, Chernogolovka, Moscow Region, 142432, Russia

$10^{30}$-$11^{00}$ **Deformation Mechanisms, Microstructure, and Mechanical Properties of High-Mn Austenitic Steels**
James Wittig
Interdisciplinary Materials Science, Vanderbilt University, Nashville, TN, USA

**Break: $11^{00}$-$11^{30}$**

**Session II: $11^{30}$-$12^{30}$**
**Chairmen: Feng-Huei Lin and Vuk Uskoković**

$11^{30}$-$12^{00}$ **Hyaluronate-based thermo-sensitive hydrogel as cell carrier for nucleus pulposus regeneration and vitreous body substitute**
Feng-Huei Lin
National Health Research Institutes (NHRI), Taipei, Taiwan

$12^{00}$-$12^{30}$ **From controlled drug delivery to gene therapies to bone regeneration: calcium phosphate nanoparticles as essential components of advanced biomaterials**
Vuk Uskoković
Department of Biomedical and Pharmaceutical Sciences, Chapman University, Irvine, CA 92618-1908, USA

$12^{30}$-$13^{00}$ **CLOSING CEREMONY**

# POSTER SESSION I

*Tuesday, September 6, 2016, $20^{00}$-$22^{00}$*

## SYMPOSIUM A: ADVANCED METHODS IN SYNTHESIS AND PROCESSING OF MATERIALS

P.S.A.1. **Novel pathway towards the synthesis of complex double perovskites**
Jasminka Popović, Marijana Jurić, Lidija Andros Dubraja, Krešimir Molcanov
Ruđer Bošković Institute, Bijenička 54, HR-10000 Zagreb, Croatia

P.S.A.2. **High-temperature treatment for new properties of $LuPO_4$:Eu, $Lu_2O_3$:Tb,Ti/Hf and $BaHfO_3$:Pr**
Justyna Zeler, Dagmara Kulesza, Ioannis Seferis, Eugeniusz Zych
Faculty of Chemistry, University of Wrocław, 14 F. Joliot-Curie Street, 50-383 Wrocław, Poland

P.S.A.3. **Processing and characterization of dental acrylate improved with zirconia**
Abdulsalam Ahmed Emadani, Nataša Tomić, Miloš Petrović, Dusica B. Stojanović, Petar S. Uskoković, Radmila Jančić Heinemann, Vesna Radojević
University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, Belgrade, Serbia

P.S.A.4. **Biocompatible poly(methyl methacrylate)/di-methyl itaconate – (iron oxide dopped alumina) composite with improved mechanical properties**
Gamal Ali Lazouzi, Nataša Tomić, Miloš Petrović, Milorad Zrilić, Vesna Radojević, Radmila Jančić Heinemann
University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, Belgrade, Serbia

P.S.A.5. **Rapid fabrication of antimicrobial poly(vinyl butyral)/ titania nanofibers using multi-needle electrospinning**
Faisal Ali Alzarrug, Dušica B. Stojanović, Vera M. Obradović, Anđela N. Radisavljević, Aleksandar M. Kojović, Petar S. Uskoković, Radoslav R. Aleksić
University of Belgrade, Faculty of Technology and Metallurgy, Serbia

P.S.A.6. **Thin films of $MoS_2$ on $Cu_2O$ as biosensors**
Alexandra Yu. Ledneva[1], Sofya B. Artemkina[1], Hsiang-Chen Wang[2], Vladimir E. Fedorov[1]
[1]Nikolaev Institute of Inorganic Chemistry, Siberian Branch of Russian Academy of Sciences, Novosibirsk, Russia
[2]Graduate Institute of Opto-Mechatronics, National Chung Cheng University, Taiwan

P.S.A.7. **PVA membranes doped with Ti and Zr oxide for alkaline electrolysis with ionic activators**

Slađana Maslovara[1], Dragana Zugić[1], Milica Marceta Kaninski[1], Vladimir Nikolić[1], Gvozden Tasić[1], Yuri Kochnev[2]
[1]Vinča Institute of Nuclear Sciences, Department of Physical Chemistry, University of Belgrade, Serbia, [2]Flerov laboratory of nuclear reactions, Joint institute for nuclear research, Dubna, Russia

P.S.A.8. **Influence of the nickel loading and the calcination temperature on the activity of NiO-$Al_2O_3$ catalyst prepared by mixing powders of metal oxides in the partial oxidation of methane**

Matilda Lazić
Technical College of Applied Sciences in Zrenjanin, Zrenjanin, Serbia

P.S.A.9. **Structural and magnetic properties of mechanochemically synthesized $LaFe_{1-x}Cr_xO_3$ (x = 0.5 and 0.75)**

Dragana Jugović[1], Ivica Bradarić[2], Čedomir Jovalekić[3], Tanja Barudžija[2], Vladan Kusigerski[2], Miodrag Mitrić[2]
[1]Institute of Technical Sciences of SASA, Belgrade, Serbia, [2]Institute of Nuclear Sciences “Vinča”, University of Belgrade, Belgrade, Serbia, [3]Centre for Multidisciplinary Studies, University of Belgrade, Belgrade, Serbia

P.S.A.10. **Surfactant-assisted high energy ball milling technique as a method for preparation of magnetic submicrometer particles**

Vesna Jović, Jelena Lamovec, Katarina Radulović, Danijela Ranđelović, Zoran Jakšić, Dana Vasiljević – Radović
Centre of Microelectronic Technologies, Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoseva 12, 11000 Belgrade, Serbia

P.S.A.11. **Characterization of NdFeB magnetic submicron particles obtained by surfactant-assisted high energy ball milling (SA-HEBM)**

Jelena Lamovec[1], Vesna Jović[1], Davor Lončarević[2], Katarina Radulović[1], Zoran Jakšić[1], Danijela Ranđelović[1], Dana Vasiljević – Radović[1]
[1]Centre of Microelectronic Technologies, Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Belgrade, Serbia, [2]Department of Catalysis and Chemical Engineering, Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoseva 12, 11000 Belgrade, Serbia

P.S.A.12. **Experimental and theoretical analysis of fullerenol nanoparticles/water system**

Milan Vraneš, Ivana Borišev, Stevan Armaković, Sanja J. Armaković, Aleksandar Tot, Danica Jović, Slobodan Gadžurić, Aleksandar Đorđević
[1]Department for Chemistry, Biochemistry and Environmental Protection, University of Novi Sad, Novi Sad, Serbia, [2]Department of Physics, Faculty of Sciences, University of Novi Sad, Novi Sad, Serbia

P.S.A.13. **Highly efficient graphene supports for fuel cells**
Veera Sadhu[1], Esaam Jamil[2], Selmiye Alkan Gürsel[1,2]
[1]Nanotechnology Research and Application Center, Sabanci University, 34956 Istanbul, Turkey, [2]Faculty of Natural Science and Engineering, Sabanci University, 34956 Istanbul, Turkey

P.S.A.14. **Modeling of optimal parameters of synthesis and sintering of nanostructured NiFeCuW powder**
Slađana Đurašević[1], Dejan Vujičić[1], Marija Nikolić[2], Siniša Ranđić[1]
[1]Faculty of Technical Sciences in Čačak, University of Kragujevac, Serbia
[2]Technical College Čačak, Serbia

P.S.A.15. **The study of the products of off-line pyrolysis of poly(ethyleneimine)**
Vesna Balanac[1], Tatjana Šolević Knudsen[2], Branimir Jovančićević[3], Jan Schwarzbauer[4], Vesna Antić[5]
[1]Cooper Standard Srbija doo, Sremska Mitrovica [2]Center of Chemistry, Institute of Chemistry, Technology and Metallurgy, Belgrade, Serbia [3]Faculty of Chemistry, Belgrade, Serbia [4]Institute of Geology and Geochemistry of Petroleum and Coal, RWTH Aachen University, Aachen, Germany [5]Faculty of Agriculture, Zemun, Serbia

P.S.A.16. **Parameters and sinterability of mullite-$ZrO_2(Y_2O_3)$ nanoparticles prepared by plasma and chemical methods**
Jānis Grabis, Dzidra Jankoviča, Inta Sīpola
Riga Technical University, Faculty of Material Science and Applied Chemistry, Institute of Inorganic Chemistry, Riga, Latvia

P.S.A.17. **Sample preparation method influence on SOP modes in ZnO(Mn)**
Branka Hadžić, Nebojsa Romčević, Maja Romčević, Witold Dobrowolski, Martina Gilić, Milica Petrović, Dusanka Stojanović, Željka Nikitović and Zorica Lazarević
[1]Institute of Physics, Belgrade, Serbia, [2]Institute of Physics Polish Academy of Science, Warzawa, Poland

P.S.A.18. **Crystal structure, optical and magnetic properties of ZnO:Fe nanoparticles**
Vladimir Rajić[1], Smilja Marković[2], Ljiljana Veselinović[2], Miodrag Mitrić[3], Jelena Belošević-Čavor[3], Valentin Ivanovski[3], Vladan Kusigerski[3], Miloš Mojović[1], Srečo Davor Škapin[4], Stevan Stojadinović[5], Steva Lević[6], Vladislav Rac[6], Dragan Uskoković[2]
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# POSTER SESSION II

*Wednesday, September 7, 2016, $20^{00}$-$22^{00}$*

## SYMPOSIUM B: ADVANCED MATERIALS FOR HIGH-TECHNOLOGY APPLICATIONS

P.S.B.1. **Electrone structure, valence state Ce(Yb) and magnetic properties of new ternary intermetallic compounds**

Ivan Shcherba[1,2], Dragan Uskokovic[3], Viktor Antonov[4], Maria Kovalska[2], Ljubov Romaka[2], Sergij Senkiv[2]

[1]Institute of Technology, the Pedagogical University of Cracow, Podchorozych st. 2 Cracow 30-084 Poland, [2]Ivan Franko National University of Lviv, Ukraine, [3]Institute of Technical Sciences of SASA, Belgrade, Serbia, [4]Institute of Physics of Metals, NASU, Kyiv, Ukraine

P.S.B.2. **Influence of different precursor solutions on final characteristics of barium titanate based thin films**

Jovana Stanojev[1], Jelena Vukmirović[1], Branimir Bajac[1], Elvira Đurđić[2], Srđan Rakić[2], Vladimir V. Srdić[1]

[1]Faculty of Technology, Department of Materials Engineering, University of Novi Sad, Bul. Cara Lazara 1, 21000 Novi Sad, Serbia, [2]Faculty of Sciences, Department of Physics, University of Novi Sad, Trg D. Obradovića 4, 21000 Novi Sad, Serbia

P.S.B.3. **YBCO bulk superconductor exposed to air moisture**

Pavel Diko[1], Mária Kaňuchová[2], Samuel Piovarči[1], Vitaliy Antal[1], Daniela Volochová[1]

[1]Institute of Experimental Physics, Slovak Academy of Sciences, Watsonova 47 04001 Košice, Slovakia, [2]Faculty of Mining, Ecology, Process Control and Geotechnology, Technical University of Košice, Park Komenského 17, 042 00 Košice, Slovakia

P.S.B.4. **Computational study of loratadine reactivity in order to understand its degradation properties from the aspect of DFT and MD simulations**

Sanja J. Armaković[1], Stevan Armaković[2] and Biljana Abramović[1]

[1]University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg D. Obradovića 3, 21000 Novi Sad, Serbia, [2]University of Novi Sad, Faculty of Sciences, Department of Physics, Trg D. Obradovića 4, 21000 Novi Sad, Serbia

P.S.B.5. **Synthesis and characterization of Pd nanocatalyst at tungsten carbide based support for fuel cells application**

Ljiljana M. Gajić-Krstajić[1], P. Zabinski[2], V.R. Radmilović[3], P. Ercius[4], M. Krstajić-Pajić[5], U.Č. Lačnjevac[6], N.V. Krstajić[3], N.R. Elezović[6]
[1]Institute of Technical Sciences of SASA, Knez Mihailova 35, Belgrade, Serbia, [2]AGH University of Science and Technology, Faculty of Non-Ferrous Metals, Al. Mickiewicza 30,30-059 Krakow, Poland, [3]Faculty of Technology and Metallurgy University of Belgrade, Karnegijeva 4, 11000 Belgrade, Serbia, [4]National Center for Electron Microscopy, LBNL University of California, Berkeley, CA, USA, [5]Institute for Chemistry Technology and Metallurgy University of Belgrade, Njegoseva 12, Belgrade, [6]Institute for Multidisciplinary Research, University of Belgrade, Kneza Viseslava 1, 11030 Belgrade, Serbia

P.S.B.6. **Corrosion stability of graphene coatings on metallic substrates**

Ivana Jevremović[1], Samira Naghdi[2], Kyong Yop Rhee[2], Vesna Mišković-Stanković[1]
[1]Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia, [2]Department of Mechanical Engineering, College of Engineering, Kyung Hee University, 446-701 Yongin, Republic of Korea

P.S.B.7. **Solid-state reactions in nanomaterials based on monolayered chalcogenides of transition metals**

Svetlana Kozlova, Maxsim Ryzhikov, Vladimir Fedorov
Nikolaev Institute of Inorganic Chemistry SB RAS, 630090, Ave. Akad. Lavrentiev 3, Novosibirsk, Russia

P.S.B.8. **SiC and Si-C-N ceramics derived from new siliconorganic polymers**

Aleksei Utkin, Natalya Baklanova
Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk, Russia

P.S.B.9. **Macroporous conducting cryogels based on polyaniline**

Jaroslav Stejskal, Miroslava Trchová, Patrycja Bober
Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, 162 06 Prague 6, Czech Republic

P.S.B.10. **Temperature responsive hydrogels with ethylene glycol propylene glycol pendant chains**

Edin Suljovrujić, Zorana Rogić Miladinović, Dejan Miličević, Maja Mićić
Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia

P.S.B.11. **Nanocomposites of polypyrrole nanotubes and noble-metal nanoparticles**
Miroslava Trchová[1], Irina Sapurina[1,2], Jaroslav Stejskal[1]
[1]Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, 162 06 Prague 6, Czech Republic, [2]Institute of Macromolecular Compounds, Russian Academy of Sciences, St. Petersburg 199004, Russian Federation

P.S.B.12. **Electrical properties of mechanically activated magnesium-titanate ceramics**
Nebojša Mitrović[1], Suzana Filipović[2], Jelena Orelj[1], Aleksandra Kalezić-Glišović[1], Slobodan Đukić[1]
[1]Faculty of Technical Sciences Čačak, University of Kragujevac, Serbia
[2]Institute of Technical Sciences of SASA, Belgrade, Serbia

P.S.B.13. **Influence of mechanical activation on the MgO-$Al_2O_3$-$SiO_2$ system with $TeO_2$**
Nataša Đorđević[1], Nina Obradović[2], Suzana Filipović[2], Darko Kosanović[2], Smilja Marković[2], Miodrag Mitrić[3], Vladimir B. Pavlović[2]
[1]Institute for Technology of Nuclear and Other Mineral Raw Materials, Bulevar Franse d'Eperea 86, 11000 Belgrade, Serbia, [2]Institute of Technical Sciences of SASA, Knez Mihailova 35/IV, 11000 Belgrade, Serbia, [3]Vinča Institute of Nuclear Sciences, University of Belgrade, Mike Alasa 12-14, 11000 Belgrade, Serbia

P.S.B.14. **Temperature dependence of thermal conductivity of two-layered graphene**
Stevo Jaćimovski[1], Dejan Raković[2]
[1]Academy of Criminalistic and Police Studies, Belgrade, Serbia
[2]University of Belgrade, Faculty of Electrical Engineering, Serbia

P.S.B.15. **The electrical resistance decay of a metalic granular packing**
Zorica M. Jakšić[1], Milica Cvetković[1], Julija. R. Šćepanović[1], Ivana Lončarević[2], Ljupka Budinski-Petković[2] and Slobodan B. Vrhovac[1]
[1]Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, Zemun 11080, Belgrade, Serbia, [2]Faculty of Engineering, Trg D. Obradovi´ca 6, Novi Sad 21000, Serbia

P.S.B.16. **Analyses of commercially and laboratory produced ODS steels**
Jarmila Degmová, Jana Šimeg Veterniková, Veronika Sabelová, Július Dekan, Milan Pavúk, Stanislav Sojak, Martin Petriska,Vladimír Slugeň
Institute of Nuclear and Physical Engineering, Slovak University of Technology, Ilkovičova 3, 812 19 Bratislava, Slovakia

P.S.B.17. **Ni-based alloys coatings for high temperature applications**
Monika Solecka, Agnieszka Kopia, Agnieszka Radziszewska, Jan Kusiński, Łukasz Cieniek
Department of Surface Engineering and Materials Characterisation, Faculty of Metals Engineering and Industrial Computer Science, AGH University of Science and Technology in Krakow, Poland

P.S.B.18. **Effects of retrogression and reaging treatments on the mechanical characteristics of alloy EN AW 7049A-T6**
Jelena Marinković, Ljubica Radović, Milutin Nikačević
Military Technical Institute, Belgrade, Serbia

P.S.B.19. **Characteristics of stress distribution in the case of singl LAP joint of two composite plates**
Abdurrahman Houssein
Alabel Algharbi University, Dean of Engineering Faculty, Zintan, Libya

P.S.B.20. **OLE of tribology effects on cup anemometer classification**
Miodrag Zlatanović[1], Ivan Popović[2]
[1]Wind Electricity doo, [2]School of Electrical Engineering, Beograd, Serbia

P.S.B.21. **Monte Carlo simulations of He+ in CF4**
Željka D. Nikitović, Zoran M. Raspopović, Vladimir D. Stojanović
Institute of Physics, Univerzity of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

# POSTER SESSION III

*Thursday, September 8, 2016, $20^{00}$-$22^{00}$*

## SYMPOSIUM C: NANOSTRUCTURED MATERIALS

P.S.C.1. **Characterization of graphite-encapsulated iron nanoparticles synthesized by milling-assisted low-pressure chemical vapor deposition**
Duygu Ağaoğulları[1], Steven Madsen[2], Ai Leen Koh[3], Robert Sinclair[2]
[1]Department of Metallurgical and Materials Engineering, Istanbul Technical University, Maslak, Istanbul 34469, Turkey, [2]Department of Materials Science and Engineering, Stanford University, Stanford, CA 94305-4034, USA, [3]Stanford Nano Shared Facilities, Stanford University, Stanford, CA 94305-4045, USA

P.S.C.2. **Structures and properties of quasi-onedimensional vanadium and niobium sulfides with Peierls distortion**
Vladimir E. Fedorov[1], Andrey N. Enyashin[2], Svetlana G. Kozlova[1], Mariia N. Kozlova[1], Maxim R. Ryzhikov[1]
[1]Nikolaev Institute of Inorganic Chemistry, Siberian Branch of Russian Academy of Sciences, Novosibirsk, Russia, [2]Institute of Solid State Chemistry, Ural Branch of Russian Academy of Sciences, Ekaterinburg, Russia

P.S.C.3. **Aqueous sol-gel route toward selected quaternary metal oxides with single and double perovskite-type structure containig tellurium**
Igor Đerđ[1], Berislav Marković[1], Jasminka Popović[2], Tobias Weller[3], Zvonko Jagličić[4,5], Željko Skoko[6], Damir Pajić[6], Christian Suchomski[3], Pascal Voepel[3], Roland Marschall[3], and Bernd M. Smarsly[3]
[1]Department of Chemistry, J. J. Strossmayer University of Osijek, Osijek, Croatia, [2]Ruđer Bošković Institute, Zagreb, Croatia, [3]Institute of Physical Chemistry, Justus-Liebig-University Giessen, Giessen, Germany, [4]Institute of Mathematics, Physics and Mechanics, Ljubljana, Slovenia, [5]Faculty of Civil and Geodetic Engineering, University of Ljubljana, Ljubljana, Slovenia, [6]Department of Physics, Faculty of Science, University of Zagreb, Zagreb, Croatia

P.S.C.4. **Thiol click chemistry on gold-decorated $MoS_2$: elastomer composites and structural phase transitions**
Peter Topolovsek[1], Luka Cmok[1], Christoph Gadermaier[1], Miloš Borovsak[1], J. Kovacb[2], Aleš Mrzel[1]
[1]Department of Complex Matter, Jozef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia, [2]Department of Surface Engineering and Optoelectronics, Jozef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia

P.S.C.5. **Positronics of sub-nanometer-structured functional materials**
Oleh Shpotyuk[1,2], Adam Ingram[3], Yaroslav Shpotyuk[4], Jacek Filipecki[1]
[1]Jan Dlugosz University in Czestochowa, 13/15, Armii Krajowej str., 42200, Czestochowa, Poland, [2]Vlokh Institute of Physical Optics, 23, Dragomanov str., 79005 Lviv, Ukraine, [3]Opole University of Technology, 75, Ozimska str., 45370 Opole, Poland, [4]Centre for Innovation and Transfer of Natural Sciences and Engineering Knowledge, University of Rzeszow, 1, Pigonia str., 35-959 Rzeszow, Poland

P.S.C.6. **Colloidal dispersions of zirconium and titanium trisulfides**
Pavel A. Poltarak[1], Anastasiia A. Poltarak[2], Mariia N. Kozlova[1], Sofia B. Artemkina[1], Vladimir E. Fedorov[1]
[1]Nikolaev Institute of Inorganic Chemistry, Russia
[2]Novosibirsk State University, Russia

P.S. C.7. **Investigation of rheological properties of barium titanate inks and adaptation to requirements of inkjet printing**
Jelena Vukmirović[1], Jovana Stanojev[1], Branimir Bajac[1], Elvira Đurđić[2], Sanja Kojić[3], Goran Stojanović[3], Srđan Rakić[2], Vladimir V. Srdić[1]
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P.S.C.8. **Sputter-deposited Fe/Al thin superlattices: scanning of non-magnetic layer thickness**
Ali Karpuz[1], Hakan Kockar[2], Salih Colmekci[2], Mehmet Uckun[2]
[1]Department of Physics, Karamanoglu Mehmetbey University, Karaman, Turkey, [2]Department of Physics, Balikesir University, Balikesir, Turkey

P.S.C.9. **Effect of IF-WS$_2$ nanoparticles addition on physical-mechanical and rheological properties and on chemical resistance of water-based paints**
Dragana Lazić, Danica Simić, Aleksandra Samolov
Military Technical Institute, Ratka Resanovića 1, 11000 Belgrade, Serbia

P.S.C.10. **Nanocrystalline boehmite obtained at low temperature**
Ivan Stijepović[1], Marija Milanović[1], Ljubica Nikolić[1], Zoran Obrenović[2]
[1]University of Novi Sad, Faculty of Technology, Department of Materials Engineering, Bulevar cara Lazara 1, 21000 Novi Sad, Serbia, [2]Faculty of Technology, University of East Sarajevo, Zvornik, Republic of Srpska, B&H

P.S.C.11. **Chromatic discretization and selectivity in optical properties of whole crystalline nanofilm-structures in IR region**

Jovan P. Šetrajčić[1], Ana J. Šetrajčić–Tomić[2], Igor J. Šetrajčić[1], Siniša M. Vučenović[3]
[1]University of Novi Sad, Faculty of Sciences, Department of Physics, Novi Sad, Vojvodina – Serbia, [2]University of Novi Sad, Faculty of Medicine, Department of Pharmacy, Novi Sad, Vojvodina – Serbia, [3]University of Banja Luka, Faculty of Sciences – Physics, Banja Luka, Republic of Srpska – B&H

P.S.C.12. **Effect of IF-WS$_2$ nanoparticles addition on thermo-rheological and mechanical behavior of aramid/phenolic resin/PVB composite material**

Danica M. Simić[1], Dušica B. Stojanović[2], Ana D. Tasić[1], Petar S. Uskoković[2], Radoslav R. Aleksić[2]
[1]Military Technical Institute, Ratka Resanovića 1, 11000 Belgrade, Serbia, [2]University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11000 Belgrade, Serbia

P.S.C.13. **Microstructure characterization of friction stir welded joints made from ultrafine grained aluminium**

Marta Lipinska[1], Lech Olejnik[2], Adam Pietras[3], Andrzej Rosochowski[4], Malgorzata Lewandowska[1]
[1]Faculty of Materials Science and Engineering, Warsaw University of Technology, Woloska 141, 02-507 Warsaw, Poland, [2]Institute of Manufacturing Processes, Warsaw University of Technology, Narbutta 85, 02-524 Warsaw, Poland, [3]Department of Friction and Resistance Welding and Environmental Engineering, Institute of Welding, Czeslawa 16/18, 44-100 Gliwice, Poland, [4]Design, Manufacture and Engineering Management, University of Strathclyde, 75 Montrose Street, Glasgow G1 1XJ, United Kingdom

P.S.C.14. **Synthesis of colloidal NIR-luminescent nanoparticles of rare-earth fluorides using microwave-hydrothermal treatment**

Alexander Vanetsev[1,2], IlmoSildos[1], Yurii Orlovskii[1,2]
[1]Institute of Physics, University of Tartu, Tartu, Estonia, [2]General Physics Institute, Russian Academy of Sciences, Moscow, Russia

## SYMPOSIUM E: BIOMATERIALS

P.S.E.1. **Synthesis, characterization and biological application of opto-magnetic nanocomposites with up-converting properties based on $NaYF_4$&$Fe_3O_4$@$SiO_2$ nanoparticles**

Przemysław Kowalik[1], Bożena Sikora[1], Krzysztof Fronc[1], Jakub Mikulski[1], Izabela Kamińska[1], Anna Borodziuk[2], Magdalena Duda[2], Katarzyna Łysiak[3], Maciej Szewczyk[4,5], Karolina Zajdel[6], Grzegorz Gruzeł[7], Leandro C. Figueiredo[8], Paulo C. Morais[8,9], Laise Andrade[10], João P. Longo[10], Ricardo B. de Azevedo[10], Zulmira G. M. Lacava[10], Ewa Mosiniewicz-Szablewska[1], Magdalena Parlińska-Wojtan[7], Roman Minikayev[1], Tomasz Wojciechowski[1], Anita Gardias[3], Jarosław Rybusiński[3], Andrzej Sienkiewicz1[1,12], Mariusz Łapiński[13], Piotr Stępień[4,5,14], Wojciech Paszkowicz[1], Jacek Szczytko[3], Andrzej Twardowski[3], Małgorzata Frontczak-Baniewicz[6], Danek Elbaum[1]
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P.S.E.2. **Development and characterization of Mg-containing hydroxyapatite, β-tricalcium phosphate and biphasic calcium phosphate bioceramics**

Liga Stipniece, Inga Narkevica, Kristine Salma-Ancane, Liga Berzina-Cimdina
Rudolfs Cimdins Riga Biomaterials Innovations and Development Centre of RTU, Institute of General Chemical Engineering, Faculty of Materials Science and Applied Chemistry, Riga Technical University, Latvia

P.S.E.3. **Design and characterization of hydroxyapatite/poly(vinyl alcohol) nanocomposite coated titania scaffolds for bone repair**

Inga Narkevica, Liga Stipniece, Jurijs Ozolins
Rudolfs Cimdins Riga Biomaterials Innovations and Development Centre of RTU, Institute of General Chemical Engineering, Faculty of Materials Science and Applied Chemistry, Riga Technical University, Pulka St. 3, Riga, LV-1007, Latvia

P.S.E.4. **Color of dental composite restorations related to dentin substituents**

Jovana Marjanović[1], Đorđe Veljović[2], Tatjana Savić-Stanković[1], Branka Trifković[3], Đorđe Janaćković[2], Vesna Miletić[1]
[1]University of Belgrade, School of Dental Medicine, DentalNet Research Group, Rankeova 4, Belgrade, Serbia, [2]University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11120 Belgrade, Serbia, [3]University of Belgrade, School of Dental Medicine, Department of Prosthodontics, Rankeova 4, Belgrade, Serbia

P.S.E.5. **Synthesis, characterization and antimicrobial activity of pentagonal bipyramidal Fe(III) complexes with 2,6-diacetyl- pyridine bis(trimethylammoniumacetohydrazone)**

Božidar R. Čobeljić[1], M.T. Milenković[2], M.R. Milenković[1], G.V. Brađan[1], D.D. Radanović[3] and K.K. Anđelković[1]
[1]Faculty of Chemistry, University of Belgrade, Studentski trg 12–16, 11000 Belgrade, Serbia, [2]Department of Microbiology and Immunology, Faculty of Pharmacy, University of Belgrade, Vojvode Stepe 450, Serbia, [3]Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 12, P.O. Box 815, 11000 Belgrade, Serbia

P.S.E.6. **Synthesis and development of polymeric scaffolds based on (meth)acrylates for tissue regeneration applications**

Jovana S. Vuković, Marija M. Babić, Bojan Đ. Božić, Katarina M. Antić, Vuk V. Filipović, Jovanka M. Filipović, Simonida Lj. Tomić
Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, Belgrade, Serbia

# Abstracts

# Oral Presentation

MRS-Serbia 2016 Award

# Cell-instructive biomaterials for tissue engineering: Applications in regenerative medicine and study of disease

Gordana Vunjak-Novaković
Columbia University, Department of Biomedical Engineering,
Laboratory for Stem Cells and Tissue Engineering, New York, NY, USA

Tissue engineering is becoming increasingly successful with authentically representing the actual environmental milieu of human development, regeneration and disease. A classical paradigm of tissue engineering involves the use of human cells, biomaterial scaffolds (structural and logistic templates for tissue formation) and bioreactors (culture systems providing environmental control, molecular and physical signaling) in regenerative medicine. Today, living human tissues can be bioengineered from autologous stem cells, and tailored to the patient and the medical condition being treated. A reverse paradigm is now emerging with the development of platforms for modeling of integrated human physiology, using iPS cell derived micro-issues of different types functionally connected by microvasculature. The biological fidelity of these “tissues on a chip” platforms and the capability for high-throughput work and real-time measurement of physiological responses are poised to transform preclinical drug screening and modeling of human disease.

The new generation of biomaterials, designed to structurally, biologically and mechanically resemble the native tissue matrix, is a key driver of progress in the research and applications of tissue engineering. This talk will discuss the common underlying principles of tissue engineering, and some recent advances in biomaterial designs. To illustrate the current capabilities and the challenges ahead, we focus on three areas of high scientific and clinical interest: bone regeneration, cardiac tissue organoids for drug testing, and modeling of solid tumors.
Funding: National Institutes of Health, New York State Department of Health, New York City Investment Fund (Bioaccelerate Program) and Mikati Foundation for Research.

PL.S.I.1.

# Stimuli-responsive smart soft materials

Takuzo Aida
The University of Tokyo and RIKEN Center for Emergent Matter Science, Tokyo, Japan

Machine technology frequently puts magnetic or electrostatic repulsive forces to practical use, as in maglev trains, vehicle suspensions or non-contact bearings. In contrast, materials design overwhelmingly focuses on attractive interactions, such as in the many advanced polymer-based composites, where inorganic fillers interact with a polymer matrix to improve mechanical properties. However, articular cartilage strikingly illustrates how electrostatic repulsion can be harnessed to achieve unparalleled functional efficiency: it permits virtually frictionless mechanical motion within joints, even under high compression. Here we describe a composite hydrogel with anisotropic mechanical properties dominated by electrostatic repulsion between negatively charged unilamellar titanate nanosheets embedded within it. Crucial to the behaviour of this hydrogel is the serendipitous discovery of cofacial nanosheet alignment in aqueous colloidal dispersions subjected to a strong magnetic field, which maximizes electrostatic repulsion and thereby induces a quasi-crystalline structural ordering over macroscopic length scales and with uniformly large face-to-face nanosheet separation. We fix this transiently induced structural order by transforming the dispersion into a hydrogel using light-triggered in situ vinyl polymerization. The resultant hydrogel, containing charged inorganic structures that align cofacially in a magnetic flux, deforms easily under shear forces applied parallel to the embedded nanosheets yet resists compressive forces applied orthogonally. We anticipate that the concept of embedding anisotropic repulsive electrostatics within a composite material, inspired by articular cartilage, will open up new possibilities for developing soft materials with unusual functions.

References:

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PL.S.I.2.

## Therapeutic biomaterial devices for controlled drug release in ocular and cardiac disease treatment

Freddy Boey, Subbu Venkatraman
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Controlled Local Drug Release through the use of Biodegradable Biomaterials has recently been shown to be a highly efficacious method for therapeutic treatment of diseases. This presentation shares the results of both the research and the commercialization aspects of some devices developed in Nanyang Technological University (NTU), l which has led to a funded startup company each. The first is the development of a fully biodegradable multi layered and drug eluting biopolymer stent for treating coronary artery blockages. The company has successfully carried out Phase 2 human trials and has attracted a buy in from a major Biomedical Device company, Boston Scientific. The second is the development of a first ever injected nanoliposome that elutes Latanoprost locally, which has been successfully shown to continuously reduce the Intra Occular Pressure for up to 6 months in its first human trials. The technology has since led to a funded startup company with funding towards Phase 2 clinical trials.

PL.S.I.3.

## Iron Oxide Nanoparticles for medical application: still a challenging task

Heinrich Hofmann
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Superparamagnetic iron oxide nanoparticles are in development for medical applications since more than 20 years. In the meantime, several products were on the market and used in clinics as contrast agent for MRI or as drug for successful treatment of anemia. For economic reasons, iron oxide as contrast agent disappeared from the market, because it was only accredited for the imaging of liver. Today the most useful development of superparamagnetic iron oxide is in the field of magnetic fluid hyperthermia. Particles injected locally into the tumor are efficient heat sources if an external alternate magnetic field is applied. To bring iron oxide nanoparticles to the clinics, the properties like saturation magnetization, magnetic anisotropy, colloidal stability, biocompatibility and especially the specific targeting has to be strongly improved. Bedside this, biological properties like biodistribution and residence time have to be adapted to the clinical needs. All this properties could only be improved, if the behavior of the particles is well understood, both from a physical as well as biological side.

In this talk, a short introduction of the state of the art will be given, followed by an analysis of the still existing gaps including some proposition how to overcome it. Focus of the talk will be the physico-chemical properties and in addition to a typically materials development, several aspects of the additional needs regarding standardization, accreditation and good manufacturing practice are included.

PL.S.I.4.

## In situ electron microscopy of energy-related thin film reactions

Robert Sinclair, Sang Chul Lee and Ai Leen Koh
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The structure of thin film materials, utilized for electro-chemical and catalytic purposes, profoundly influences their properties and effectiveness. Changes in structure which are brought about by heating or exposure to gaseous environments can be studied by in situ high resolution electron microscopy. This paper will show results on the reduction of amorphous molybdenum sulphide thin films in a hydrogen environment and on the behavior of ceria thin films grown epitaxially on various oxide single crystal substrates. The utility of an aberration-corrected, environmental transmission electron microscope coupled with fast image recording will be emphasized.

PL.S.I.5.

## Lithium and scandium trialuminides embedded in solid matrix

Velimir R. Radmilović
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In this presentation we will discuss formation of core/shell ordered L12 $Al_3(LiSc)$ trialuminide precipitates embedded in Al-rich matrix by solid-state reaction using multi-stage heat treatment. The conventional high-resolution imaging reveals the fully ordered structure of the shell. High angel annular dark field scanning transmission electron microscopy (HAADF), energy filtered transmission electron microscopy spectrum imaging (EFTEM-SI) and field-ion microscopy (FIM) indicates that Sc is confined to the core, while Li is predominantely confined to the shell. The chemical composition of the core region is $Al_3(Li_{0.40}Sc_{0.48}Al_{0.12})$, for which the mean atomic scattering factor of the Li, Sc, Al sublattice in the fully ordered L12 structure is very similar to that of Al. This explains why the contrast in the core is very similar to the contrast in the surrounding Al-matrix and how it is related to vanishing superlattice reflections. The presence of Li in the core is thermodynamically favorable. The phase of the exit wave reveals long-range order of the shell, in which Al columns can be distinguished easily from Li columns. Our approach demonstrates that using differential diffusivities and solubility of Li and Sc in an Al matrix it is possible to create monodisperse distribution of L12 ordered precipitates with exceptional resistance to coarsening.

O.S.F.1.

## Materials research in Europe – a new concept needed?

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Materials are classified into metals, polymers, ceramics and their various composites, and new developments such as carbon-based materials arise to be used in new innovative products. Regarding their application, materials are related to industrial sectors such as energy, health, transport, communication, construction etc. These sectors require certain functions independent on what kinds of materials and processes were used.  Such functions or “smart” properties should also meet other requirements of the end-user related to legislation, standards, ecological impact, and to the pricing on the market.

Highly innovative products contain a variety of different elements and sophisticated technologies. Materials research has enabled various breakthroughs which led to marketable innovations and improvements for climate, health and energy projects.

However, many of these innovations need more and more materials functions, and a broad variety of raw materials – amongst them materials which are critical in view of their resource availability, mining conditions, ecological footprint, social exploitation and the end of the production cycle. Most of these materials do not origin from Europe, their manufacturing makes it difficult or even impossible to recycle them, the raw materials can become expensive or are not in line with legislation e.g. for environmental standards. Materials research and development should be understood in a “whole value chain approach” which considers these aspects already in a very early phase - the invention and design stage.

Research is a first step on a way to an innovative product and happens around 10 to 15 years before the product comes on the market. Materials scientists and engineers should be aware of the challenges in each of the process steps that a product passes from mining to end-of-life to ensure long-term availability and sustainability. This presentation deals with some examples of innovative products to highlight the dependency on critical materials and shows how a “whole value chain approach” could help to develop more sustainable materials.

O.S.F.2.

## Hybrid-interface materials

Kwang Ho Kim[1,2]
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Hybrid interface technology is to form the connection in electronic, atomic, molecular and structural level among different kind of materials so that new function of materials and/or components can be revealed, and it is to create the future materials of high-performance, hybrid-function and a new feature through design-syntheses-evaluation of interface volume and composition.  In this talk, the idea and successful developments for new materials, based on our research paradigm will be introduced.

O.S.F.3.

## Advanced nanotechnology based on the directed self-assembly of block copolymers for device applications

Woon Ik Park, Jung-Ho Cho, Young Hun Jeong, and Jong Hee Whang
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The directed self-assembly (DSA) of block copolymers (BCPs) have attracted enormous attention due to its outstanding ability to overcome the challenges of conventional nanofabrication technologies. The self-assembly of BCP which consists of two or more incompatible blocks, can produce periodic patterns with sub-20 nm such as dot, line, hole and ring patterns. However, the self-assembled nanostructures are non-functional in general; therefore, they are used mainly as etch-masks or lift-off templates for producing functional nanostructures such as magnetic dots, phase-changing dots, or silicon nanowires. In this talk, for the realization of direct pattern formation with functionality, the novel and practical nanotechnology based on the directed self-assembly of block copolymer, for example, nano/micro pattern transfer printing will be introduced for next-generation nanolithography.

O.S.F.4.

## Virus based novel colorimetric sensor for cancer cell detection

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Color sensor like pregnancy test kit or litmus paper for pH test relies on color change depending on various chemical and physical conditions. Recently, we developed the novel colorimetric sensor which is functionalized with M-13 bacteriophage-based structure color [1], and it could detect TNT down to 300 p.p.b. over similarly structure chemicals [2]. Cancer cells release abnormal gas composition compared with that of normal cells. Therefore, cancer can be diagnosed by breath testing for a unique composition of volatile gas produced by each species of cells. Here, we developed the novel cancer recognition sensor suing virus-based structural color matrix. Due to its liquid crystalline behavior and surface modification ability, M-13 bacteriophage based color sensor exhibited remarkable selectivity and sensitivity to target samples including chemicals which compose VOCs of NCI. Upon exposure of small amounts of target molecules, the resulting colored matrices exhibited distinct different color changes that can be applied to effectively discriminate the target. Although the cancer cell sensing system was used as proof-of-concept in this study, this approach can be generalized to the detection of many harmful and biological toxicants.

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O.S.F.5.

## Organic-inorganic hybride thin films using atomic/molecular layer deposition for flexible electronic applications

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Nowadays, atomic layer deposition (ALD) has been a conventional deposition technique since it first invented in1974. After 1990's, the micro/nano electronics may provide ALD evolutions because ALD has unique properties such as conformal, uniform, accurate, and pinhole-free films. Recently, functional oxide and organic thin films, deposited by ALD/MLD (Molecular Layer Deposition) have been demonstrated in emerging applications (flexible, transparent, and wearable things). In this talk, I will talk the brief ALD and MLD concept, including birth, revival, and future. Then, I will show some emerging applications such as transparent conducting oxide, oxide semiconductor, and gas diffusion barriers, in terms of inorganic and organic thin films. This talk will be helpful and valuable for audience to understand ALD and MLD basics and applications.

O.S.F.6.

## Ultrathin ALD interfacial layer for improved materials properties

Zhixin Wan, Woo-Jae Lee, Kwang-Ho Kim, and Se-Hun Kwon
School of Materials Science and Engineering, Pusan National University, Republic of Korea

Atomic layer deposition (ALD) has been regarded as one of the most promising thin film deposition technique in the nanotechnology. The benefits of ALD includes the precise thickness controllability, excellent step coverage in the complex structure, excellent uniformity over large areas, and superior film properties even at a low growth temperature. Due to these benefits of ALD, it has been adopted as a key technology for the various industries such as a semiconductors, microelectronics, etc. The application of ALD is now expanding to other industries due to the continuous efforts to optimize and design new equipment processes, new precursors, and material design.

Herein, we demonstrate some examples, where ALD-based ultrathin interfacial layers were used to improve the materials properties. Examples include the development of highly corrosion resistive thin films for the protection the underlying materials against harsh environments.

O.S.F.7.

## 3-Dimensional hybrid nanostructures: Novel fabrication strategies and applications

Yeon Sik Jung
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Despite their high demand and various promising applications, the fabrication of 3D nanostructures is not straightforward. We suggest that nanotranfer printing (nTP) may be a more practical solution controllably build 3D nanostructures. An nTP technique is usually composed of several steps - preparation of nanostructured elastomeric replica, deposition of functional materials, and transfer of functional nanostructures. The nanostructures can be transferred onto other substrates by contacting the mold on the surface of the receiver substrate. To overcome the issues of resolution limit (typically several tens of nm) and low transfer yield of conventional nTP, we developed and demonstrated that solvent-assisted nanotransfer printing (S-nTP) can controllably generate extremely fine (down to sub-10 nm) functional nanostructures with excellent transfer yield (~100%). The excellent uniformity of the printed nanostructures is another advantage of nTP, as it makes it possible to obtain highly uniform and reproducible 3D nanostructures composed of different materials. In this talk, we will introduce several applications of 3D hybrid nanostructures such as platinum nanocatalysts with outstanding performances and durability and plasmonic nanostructures for surface-enhanced Raman spectroscopy.

O.S.F.8.

## Hybrid materials/device enabling high energy and power densities along with robust cycle life

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Department of Materials Science & Engineering and Graduate School of EEWS,
Daejeon, Republic of Korea

Nanocrystals are promising structures, but they are too large for achieving maximum energy storage performance. We show that the molecular/atomic-scale energy storages lead to high-performance available via the reactions of ions to the molecule/atom energy storage sites. Furthermore, the performance of an assembled full-cell energy storage or conversion device will be presented and discussed.

O.S.F.9.

# Multi-scale computational design of active and durable materials for renewable energy systems

Byungchan Han, Joonhee Kang, Jeemin Hwang, Seunghyo Noh, Choa Kwon
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Using density functional theory (DFT) calculations and statistical formalisms we rationally design high functional materials for renewable energy systems of fuel cell, Li-ion and Li-air batteries. In the first part of the talk, we screen hundreds of alloys to identify the best candidate of non-precious nanocatalyst with ternary compounds for active oxygen reduction reaction (ORR) in fuel cell application. Our results indicate that nanoscale 3d-transition metal core encapsulated by N-doped carbon-shells can be designed as the catalyst better than conventional Pt showing excellent electrochemical stability in acidic media.

Using density functional theory (DFT) calculations and statistical formalisms we rationally design high functional materials for renewable energy systems of fuel cell, Li-ion and Li-air batteries. In the first part of the talk, we screen hundreds of alloys to identify the best candidate of non-precious nanocatalyst with ternary compounds for active oxygen reduction reaction (ORR) in fuel cell application. Our results indicate that nanoscale 3D-transition metal core encapsulated by N-doped carbon-shells can be designed as the catalyst better than conventional Pt showing excellent electrochemical stability in acidic media.

The second part of this presentation demonstrates that catalytic activities towards oxygen reduction and evolution reactions (ORR and OER) in a Li–$O_2$ battery can be substantially improved with graphene-based materials. We accomplish the goal by calculating free energy diagrams for the redox reactions of oxygen to identify a rate-determining step controlling the overpotentials. We unveil the catalytic performance is well described by the adsorption energies of the intermediates $LiO_2$ and $Li_2O_2$ and propose that graphene-based materials can be substantially optimized through either by N doping or encapsulating Cu(111) single crystal. Furthermore, our systematic approach with DFT calculations applied to design of optimum catalysts enables to screen promising candidates for the oxygen electrochemistry leading to considerable improvement of efficiency over a range of renewable energy devices. These two results are outstanding examples showing how to screen desired materials with more than single properties using combined multi-scale computations, which are validated by experimental measurements.

O.S.F.10.

# $Ni_2Si$ silicide wire fabrication by conventional metal alloy processing

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We report that a single crystal $Ni_2Si$ nanowire (NW) of intermetallic compounds which was candidate materials as interconnectors of semiconductor devices can be reliably designed using simple three-step processes: casting a ternary Cu-Ni-Si alloy, nucleate and growth of $Ni_2Si$ NWs as embedded in the alloy matrix via designing discontinuous precipitation (DP) of $Ni_2Si$ nanoparticles and thermal aging, and finally chemical etching to decouple the $Ni_2Si$ NWs from the alloy matrix. By direct application of uniaxial tensile tests to the $Ni_2Si$ NW we characterize its mechanical properties, which were rarely reported in previous literatures. Using integrated studies of first principles density functional theory (DFT) calculations, high-resolution transmission electron microscopy (HRTEM), and energy-dispersive X-ray spectroscopy (EDX) we accurately validate the experimental measurements. Our results indicate that our simple three-step method enables to design brittle $Ni_2Si$ NW with high tensile strength of 3.0 GPa and elastic modulus of 60.6 GPa.

O.S.F.11.

# Developing multi-component coatings for structural applications by a hybrid HIPIMS technique

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To increase the lifetime and performance of cutting/forming tools and machine parts/components, there are increasing demands for coatings. Coatings for structural applications require combinations of properties such as a relatively high hardness, good adhesion, wear and oxidation resistance. To fulfill these requirements, new coating materials and new synthesizing methods are needed to be developed.

In recent years, high power impulse magnetron sputtering (HIPIMS) technique has been developed as a new physical vapor deposition technique. By utilizing a very high power density at the target at a very short time, HIPIMS process, is achieving a high degree of ionization of the sputtered species, which opens significant opportunities for substrate-coating interface engineering and tailoring coating growth and resulting properties. The HIPIMS technique can be utilized to obtain dense coatings with high hardness and low-level residual stress. These characteristics make this technique desirable in synthesizing hard coatings. Especially, if combined with other sputtering sources, multi-component coatings for hybrid functions can be synthesized.

In this presentation, some multi-component coatings, such as MeAlSiN (Me= Ti, Cr), Me-B-N, $Ti_2AlN$ for structural applications were developed by a hybrid HIPIMS technique. The related coating microstructure and properties will be presented.

PL.S.II.1.

# In situ off-axis electron holography of two-dimensional transition metal dichalcogenides

Rafal E. Dunin-Borkowski[1], Florian Winkler[1], Amir H. Tavabi[1], Juri Barthel[2],
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Transition metal dichalcogenides (TMDs) have attracted much attention in recent years due to their enormous potential for applications in nanoelectronic devices. However, the electrical properties of mono- or few- layer TMDs can be influenced strongly by the presence of dopants, contamination and defects, as well as by their interfaces to three-dimensional metal contacts. Here, we present high-resolution off-axis electron holography measurements of the electron wavefunction that has passed through ultra-thin flakes of $WSe_2$. We show that the combined analysis of phase and amplitude from experimental electron holograms and corresponding simulations allows an accurate determination of the local specimen thickness, as well as the determination of a value for the mean inner potential of $WSe_2$ of 18.9±0.8 V, which is 12% lower than the value calculated from neutral atom scattering factors. We also present preliminary electrical biasing experiments carried out on individual TMD flakes in situ in the transmission electron microscope. Electrical contacts are patterned using electron beam lithography on a SiN membrane. In order to provide a vacuum reference wave for off-axis electron holography, the TMD flakes are partly suspended over holes in the SiN membrane.

PL.S.II.2.

## Real-time viewing of III-V semiconductor nanowire growth by In Situ TEM

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Semiconductor nanowires (NWs) and nanopyramids have a clear potential for areas like optronics, wrap-gate FETs, solar cells and efficient white LEDs. However some hurdles must be passed on the way. Lattice misfit, which causes severe dislocations, is one of the major obstacles when growing thin layers on substrates. For LED:s based on III-nitrides, intended to fill “the green gap”, we will show that this obstacle can be overcome by growth through nanoscale apertures, forming nanopyramids with high perfection. Another way to overcome the lattice misfit is to grow 1-D nanowires. Nanowires can accept much larger misfits and metal nanoparticle catalyzed growth by MOCVD has been a very successful approach to build nanoelectronics and devices with the high accuracy needed for full scale production. Recently, a new method for growth, Aerotaxy[1] has been invented, which eliminates the need of expensive substrates and allows much higher growth rates than epitaxial growth. Theoretical modeling for Aerotaxy growth is still largely undeveloped, which is why observation of growth on the atomic scale, while varying parameters like temperature, pressure and ratio of the III and V element precursor gases is most helpful[2]. We will show preliminary results from an in-house constructed closed cell[3] as well as a dedicated Environmental TEM, based on a 300 kV FEG with an aplanatic image aberration corrector. A gas supply system will deliver 9 different gases at the specimen area with a pressure of at least 1 Pa, and the specimen area can be heated to >700ºC.

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PL.S.II.3.

# Oxidation of carbon nanotubes using environmental TEM and the influence of the imaging electron beam

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Carbon nanotubes (CNTs) can be used as field emission electron sources in X-ray tubes for medical applications [1, 2]. In a laboratory setting, field emission measurements of CNTs are usually carried out in an ultra-high vacuum system with base pressure of about $10^{-7}$ mbar or better. Under less stringent vacuum conditions, CNTs are found to exhibit lower emission currents and reduced lifetimes [3, 4].

Here, we report the direct study on the structural changes in CNTs as we heated and oxidized them in situ using an aberration-corrected environmental TEM [5]. We established a protocol whereby heating and oxidation were performed without an imaging beam and changes on identifiable nanotubes were documented after purging the gas from the chamber, to ensure that they were due to the effect of gaseous oxygen molecules on the nanotubes, rather than the ionized gas species [5]. Contrary to earlier reports that CNT oxidation initiates at the end of the tube and proceeds along its length, our findings show that only the outside graphene layer is being removed and, on occasion, the interior inner wall is oxidized, presumably due to oxygen infiltrating into the hollow nanotube through an open end or breaks in the tube [5]. The CNT caps are not observed to oxidize preferentially [5, 6].

In the environment of an ETEM, interaction between fast electrons and gas leads to ionization of gas molecules and increased reactivity. It is very important to evaluate the results to determine or ameliorate the influence of the imaging electron beam. We found that there is a two orders of magnitude difference in the cumulative electron doses required to damage carbon nanotubes from 80 keV electron beam irradiation in gas versus in high vacuum [7]. We anticipate that experimental conditions that delineate the influence of the imaging electron beam can be established, which will enable us to study the CNT field emission process in situ in an ETEM.

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PL.S.II.4.

# Electric field and thermal induced effects in nanostructured materials revealed by advanced in situ electron microscopy

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Transport of matter and charges as well as heat spread properties are determined by the fine scale microstructure. In situ electron microscopy enables experiments where the local properties can be directly correlated to material structure using specimen holders that are designed to enable different stimuli. We can study, for example, electric field and thermal induced changes of charge and matter transport properties and mechanisms. The direct correlation on the small scale involving individual interfaces, defects and atoms provides access to new information about which microstructural constituents that are active in determining the material properties on the macro, micro, nano and atomic scale. This talk addresses examples of in situ electrical and thermal studies.

Heating of a transmission electron microscopy (TEM) specimen can be performed in several parallel modes and this talk will address three types of heating modes and show experimental results from nanostructured materials. One mode is by resistive heating of a ring shaped support in contact with the circumference of the entire TEM sample. An additional mode is by use of a heating wire patterned on the TEM sample where the wire is contacted by leads fed through the TEM sample holder. The third mode is by active Joule heating of the nanostructure of study, such as carbon nanotubes, graphene, or metal nanowires. The purpose of having several parallel modes of heating is to enable the separation of temperature dependence, effects of self-Joule heating, effects of radiative heating and thermal transport. It is also important to be able to extract the three dimensional information about the geometry of the investigated structures.

The talk will also address electrical transport and coupling mechanisms, for example, reduced graphene oxide, metallic oligomers and nanowires. The electrical probing is performed using an in situ probe that is positioned with a sub-Ångström precision in the x-, y- and z-direction. Further functionalities are provided by patterning electrodes on the specimen. Different effects induced by electric fields will be presented.

PL.S.II.5.

# Energy loss spectroscopy at high resolution: Applications to functional oxides and nanostructures

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Electron energy loss spectroscopy (EELS) is an invaluable technique to study the detailed structure and the chemical state of materials at unprecedented spatial resolution in the Transmission Electron Microscope (TEM). Today, this technique is used to characterize nanoscale materials used in a myriad of applications from energy storage and conversion, to solid-state devices. This technique also has the potential to provide insight into much more fundamental problems where the valence state of atoms and their location is of fundamental importance. In this presentation, I describe recent developments in EELS and TEM showing that is possible to probe the changes in bonding and coordination of atoms on surfaces of oxides, and detect small lattice distortions in nanowires with quantitative imaging. I will show that, with atomic resolution EELS, it is possible to determine ordering of cations in oxides, changes in bonding in high-T superconductors and understand the performance and degradation of catalyst materials.

PL.S.II.6.

# Non-planar nanostructures at atomic scale

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Technology at the nanoscale has become one of the main challenges in science as new physical effects appear and can be modulated at will. Superconductors, materials for spintronics, electronics, optoelectronics, chemical sensing, and new generations of functionalized materials are taking advantage of the low dimensionality, improving their properties and opening a new range of applications. As developments in materials science are pushing to the size limits of physics and chemistry, there is a critical need for understanding the origin of these unique physical properties (optical and electronic) and relate them to the changes originated at the atomic scale, e.g.: linked to changes in (electronic) structure of the material.

During the lecture, I will show how combining advanced electron microscopy imaging with electron spectroscopy, as well as cathodoluminescence in an aberration corrected STEM will allow us to probe the elemental composition and electronic structure simultaneously with the optical properties in unprecedented spatial detail.

The lecture will focus on several examples in advanced nanomaterials for optical and plasmonic applications. In this way the latest results obtained by my group on direct correlation between optical properties at sub-nanometer scale and structure at atomic scale will be presented. The examples will cover a wide range of nanomaterials: quantum structures self-assembled in a nanowire: quantum wells (2D), [1,2] quantum wires (1D) [3] and quantum dots (0D) [4,5] for optical applications (LEDs, lasers, quantum computing, single photon emitters) [6,7], nanomembranes and 2D sheets [8,9]; as well as metal multiwall nanoboxes and nanoframes [10] for 3D plasmonics.

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PL.S.II.7.

# The art and science of spatially-resolved determinations of local composition in an aberration-corrected electron microscope

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The combination of x-ray energy dispersive spectroscopy (XEDS) and/or electron energy loss spectroscopy (EELS) with aberration-corrected (S)TEM has provided, in principle (tantalizingly!), the ability to determine the chemical composition of the atoms in specific atomic columns in thin foils. This has resulted in the publication of a number of reports of such determinations. However, there are a number of factors that work against the possibility of deducing accurate values for atomically-resolved compositional determinations. These include probe delocalization, spectral contributions from phonon-scattered electrons (cross-talk), beam convergence, radiation damage, and foil thickness. The influence of these various factors will be considered and an assessment made of the possibility of performing such compositional determinations. In these latter experiments, a “standard” sample is utilized, namely the B2 intermetallic compound Ni-50.4at.%Al, in which the compositions of atomic columns when viewing along <100> are known without ambiguity.

O.S.C.1.

# Structural characterization of organic bulk heterojunction solar cells

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It is an undisputed fact that conventional energy sources on this planet are limited and since solar energy has an inexhaustible power source, as well as renewable energy source, it is fairly obvious where the potential for energy production technology in the future lies. In addition, solar cell technology supports the global trend to reduce green house gases, one of the most serious problems presently facing mankind. Although the photovoltaic market is still dominated by crystalline silicon solar cells there is a rising demand for thin film devices which has sparked extensive research in the field of organic solar cells - photovoltaic devices based on organic semiconductors. These cells present a very attractive area of research because of their ability to fulfill industry demands like flexibility and simple/cost efficient processing. A way to circumvent the Shockley–Queisser efficiency limit of organic solar cells is to introduce the tandem (multi-junction) concept which constitutes stacking of two or more sub-cells with different band-gap photoactive materials which allows complementary absorption of wider spectral wavelength ranges of incident light. This study focuses on the microstructural characterization of double- and triple-junction organic solar cells using electron microscopy.

O.S.C.2.

# High-performance Ni-GDC nanocomposite anode fabricated from GDC nanocubes for low-temperature solid-oxide fuel cells

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Gadolinium-doped ceria (GDC) nanocubes with highly reactive {001} facets were synthesized as an anode material for solid-oxide fuel cells by organic-ligand-assisted hydrothermal treatment with a water-soluble amino acid, 6–amino hexanoic acid (AHA). An aerosol technique was applied to fabricate a NiO–GDC nanocube composite with water as a green solvent. The NiO–GDC nanocube composite was easily sintered even at a temperature of 1100 °C, while the conventional NiO–GDC composite covered with the most stable {111} facets was sintered at 1300 °C. Sintering at such a low temperature inhibited undesirable coarsening of NiO and GDC particles, resulting in an enlarged, triple-phase boundary (TPB). The NiO–GDC nanocube composite anode with the enlarged TPB exhibited a rather low area specific resistance compared with the conventional NiO–GDC composite anode's resistance when operated at 600 °C [1]. In addition, a core–shell anode consisting of nickel–gadolinium-doped-ceria (Ni–GDC) nanocubes was directly fabricated by a chemical process in a solution containing a nickel source and GDC nanocubes covered with highly reactive {001} facets. The cermet anode effectively generated a Ni metal framework even at 500 °C with the growth of the Ni spheres. Anode fabrication at such a low temperature without any sintering could insert a finely nanostructured layer close to the interface between the electrolyte and the anode. The maximum power density of the attractive anode was about 100 $mW\cdot cm^{-2}$, which is higher than that of a conventional NiO–GDC anode prepared by an aerosol process at 55 $mW\cdot cm^{-2}$ and 600 °C, followed by sintering at 1300 °C [2].

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O.S.C.3.

# The chemical recycling of polycarbonate using $CeO_2$ nanocatalysts

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A novel catalytic property of $CeO_2$ and its nanoparticles is discovered, and a simple chemical recycling technique for the conversion of plastic (polycarbonate) materials to their contexture monomers under hydrothermal conditions in the presence of heterogeneous $CeO_2$ catalyst using a batch reactor is proposed. The plastic material is completely depolymerized under these conditions in the presence of bulk $CeO_2$ crystal at 200 °C for 5 h. When $CeO_2$ nanoparticles approximately 6 nm in diameter are used, the catalyst amount, reaction temperature, and time required to completely depolymerize the plastic material are reduced compared with the experimental conditions using bulk crystal; the maximum monomer (bisphenol A) yield is approximately 90%. The depolymerization reaction of the plastic material correlates directly with the surface-to-volume ratio. Further decomposition of the monomer is inhibited by reducing and/or controlling the amount of the catalyst, reaction temperature, and time.

O.S.C.4.

# Modification of the materials properties via surface structuring

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Study of the functional materials used for the telecommunications, solar energy and gas storage systems are required to find an effective method in order to improve the spectral, mechanical, conducting, etc., characteristics. At present time the basic knowledge collected from the complicated area of the structuration process of the inorganic materials has indicated namely the laser method to improve dramatically the materials parameters. Our own steps in this direction have been shown in the papers [1-4] on last three years.

In the current paper the effect of the carbon nanotubes laser deposition influence on the spectral and refractive parameters of some inorganic materials will be shown. The increase of the transparency, microhardness, wetting angle, as well as the change of the refractive index will be discussed. Moreover, the decrease of the resistivity of the ITO-coating treated with the surface electromagnetic waves will be shown under the conditions when CNTs has been placed on the substrate using different electric field from 100 to 600 V/cm. Analytical and quantum-chemical simulation will support the data obtained.

The presented results are coincided with some research directions of the Lab for Photophysics of media with nanoobjects and they have been partially supported by Russian Foundation for Basic Research, grant No.13-03-00044 (2013-2015) as well as by FP7 Marie Curie International researchers exchange proposal “BIOMOLEC” (2011-2015).

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O.S.C.5.

# Half Heusler thermoelectics $Ti_{(1-x)}Fe_{(1.33+x)}Sb$ - TiCoSb

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Phase relations in the ternary system Ti-Fe-Sb have been reinvestigated. The half Heusler phase previously reported in the literature[1], $Ti_{(1+x)}FeSb$ ($-0.2 < x < 0.27$ at 800°C), has been found at a different concentration: $Ti_{(1-x)}Fe_{(1.33+x)}Sb$ ($-0.099 < x < 0.168$ at 800°C) requesting a reinvestigation of its thermoelectric behavior. In addition thermoelectric properties (TE) were studied along four isopleths $Ti_{(1-x)}Fe_{(1.33+x)}Sb$, $TiFe_{(1.33)}Sb$-TiCo-Sb, $TiCo_{(0.5)}Fe_{(0.665)}Sb$-$TiCoSb_{(0.75)}Sn_{(0.25)}$ and $TiCo_{(0.75)}Fe_{(0.33)}Sb$- $TiCoSb_{(0.75)}Sn_{(0.25)}$ in the temperature range from 300 K to 850 K by measurements of the electrical resistivity (rho), the Seebeck coefficient (S) and the thermal conductivity (lambda) from which the dimensionless figure of merit (ZT) was calculated. Composition dependences for the TE properties for these series were developed. It was shown that p-type $Ti_{(1-x)}Fe_{(1.33+x)}Sb$ shows a semi-conducting like behavior for the Fe-rich composition ($x=0.168$) but the conductivity type changes to metallic with increase of the Ti content in this compound. The highest ZT=0.3 at 800 K in this series was found for the composition $TiFe_{(1.33)}Sb$. It was established that the TE performance also increases with Fe/Co substitution and reaches a values of ZT=0.42 for $TiCo_{(0.5)}Fe_{(0.665)}Sb$. No further increase of the TE performance was obtained for Sb/Sn substituted compounds from the sections: $TiCo_{(0.5)}Fe_{(0.665)}Sb$-$TiCoSb_{(0.75)}Sn_{(0.25)}$ and $TiCo_{(0.75)}Fe_{(0.33)}Sb$-$TiCoSb_{(0.75)}Sn_{(0.25)}$, however, it could be shown that the ZT values were enhanced by about 12 % via optimization of the preparation route (ball-milling conditions and heat treatments). In order to study compatibility of metal electrodes also the system Ti-Sb has been elucidated from DTA, X-ray diffraction and electron probe micro-analyses.

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O.S.C.6.

# Shape directing agents for controlling the morphology of anisotropic iron oxide nanoparticles

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The design and synthesis of anisotropic iron oxide nanoparticles (IONPs) of different sizes has received considerable attention because of their shape dependent magnetic properties and their diverse applications in biomedicine, separation, energy storage and sensing devices, etc. Thus, the aim of the present study is to investigate the evolution of anisotropic IONPs of tunable morphology in the presence of individual and mixture of surfactants. IONPs of cubic morphology are formed in the presence of oleic acid (OA). The morphology of NPs changes to truncated octahedra when the secondary surfactant (i.e., Tridodecylmethyl ammonium iodide, TDAI) was introduced to the reaction mixture. In the presence of oleylamine (OAm) together with TDAI and OA, we observed the growth of even more complex structures, i.e., multiple twinned NPs possessing fivefold symmetry, observed in magnetite for the first time. Magnetic properties of different shaped NPs have also been measured and compared.

Acknowledgements: This work was supported by MagBioVin ERA Chair project that received funding from European Union’s Seventh Framework Program for research, technological development and demonstration (2014-2019), COST Action MP1308 Towards Oxide-Based Electronics (TO-BE) and NanoLab fascilities of NTNU, Trondheim, Norway.

O.S.E.1.

# Multifunctional opto-magnetic NaYF$_4$:Er$_{3+}$,Yb$_{3+}$,Gd$_{3+}$&Fe$_3$O$_4$@SiO$_2$ nanoconstructs – towards biomedical applications

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Each year 8 million people die of cancer. This number is predicted to rise to 13.2 million in 2030. There is a growing interest in improving the existing modalities for early diagnosis and minimally-invasive cancer treatment, such as photodynamic diagnosis (PDD) and therapy (PDT). This proposal addresses the major current shortcoming of PDD/PDT, i.e. the inaccessibility of deep-lying tumours, by designing near infrared (NIR) light-active multifunctional optomagnetic nanocomposites (NCs). The proposed NCs will combine optical imaging and photosensitization of reactive oxygen species (ROS) under NIR light illumination with magnetic properties, thus enabling NIR-light stimulated PDD/PDT, magnetic field-driven tissue targeting, enhanced contrast in magnetic resonance imaging (MRI), as well as hyperthermia treatment. Beta-NaYF4-based upconversion nanophosphors (UCNPs) codoped with rare earth ions were synthesized. UCNPs were encapsulated with superparamagnetic Fe$_3$O$_4$ iron oxides (SPIONs) in SiO$_2$ shells, thus forming multifunctional NCs, UCNPs&SPIONs@SiO$_2$. The photocatalytic properties were assured by functionalization with photosensitizers.

In this work, we sensitized opto-magnetic multifunctional nanoconstructs based on rare earth ions – doped β-NaYF$_4$ nanoparticles, having sizes < 20 nm and revealing a high UCL efficiency. These β-NaYF$_4$ nanoparticles were co-encapsulated in SiO$_2$ with superparamagnetic Fe$_3$O$_4$ nanoparticles, thus leading to the formation of UCNPs&SPIONs@SiO$_2$ nanoconstructs. The thorough characterization confirmed that UCNPs&SPIONs@SiO$_2$ nanoconstructs combine the capability of NIR-to-VIS light up-conversion with useful superparamagnetic properties. We also demonstrated that, under illumination with NIR light, the UCL emission of rare earth ions – doped β-NaYF$_4$ efficiently excited molecules of selected photosensitizers (e.g. Rose

Bengal, Methylene Blue, hematoporphyrin, silicon phthalocyanine dihydroxide), towards ROS generation. The ROS generation was measured with optical spectroscopy and electron spin resonance (ESR).

The hyperthermia effects due to the superparamagnetic properties of SPIONs was measured as a function several experimental parameters, including: the time of application of AMF, the size and concentration of nanoparticles, as well as the type of the solvent. The intrinsic loss power (ILP) factor was determined.

Toxicity remains one of the fundamental issues concerning biological and medical application of advanced materials. Therefore, we tested our nanoconstructs in living HeLa and HEK293 cells using commercial viability tests, i.e. MTT and Presto Blue assays. We demonstrated that the opto-magnetic nanoconstructs are relatively non-toxic and are, therefore, potentially useful for selected medical applications.

Acknowledgements: The research was partially supported by the project „Development of the cluster center of biomedical engineering” implemented under Economy Operational Program (project no. UDA-POIG.05.01.00-00), the EU Research Project FP7-People-2012-IRSES-BRASINOEU (Grant Agreement Number: PIRSES-GA-2012-318916), the grants of PNSC 2013/11/B/NZ1/00089, NN UMO-2013/08/A/ST3/00297, DEC-2012/07/B/ST5/02080 and DEC-2014/15/D/ST5/02604. This work has been done in the NanoFun laboratories co-financed by the European Regional Development Fund within the Innovation Economy Operational Program, the Project No. POIG.02.02.00-00-025/09/. This research was also co-financed by the Swiss National Science Foundation through the Nano-Tera.ch Focused Project (NTF), ‘NanoUp’

O.S.E.2.

# Tumor-selective hybrid system based on hydroxyapatite nanocarrier, chitosane, poly(lactic-co-glycolic acid) and androstan derivate

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The applicative potential of synthetic calcium phosphates, especially hydroxyapatite (HAp), has become intensely broadened in the past 10 years, from bone tissue engineering to multiple other fields of biomedicine. Previously we have shown that hydroxyapatite nanoparticles coated with chitosan-poly(D,L)-lactide-co-glycolide (HAp/Ch-PLGA) target lungs following their intravenous administration into mice. For this purpose radioactive 125-Iodine (125I), a low energy gamma emitter, was used to develop a novel in situ method for radiolabeling of particles and investigation of their biodistribution.

In this study we utilize an emulsification process and freeze drying to load the composite particles based on hydroxyapatite nanocarrier, chitosane and poly(lactic-co-glycolic acid) with 17β-hydroxy-17α-picolyl-androst-5-en-3β-acetate (A), a chemotherapeutic derivative of androstane. The picolyl androstane derivatives showed high potency in the cell inhibitors of hormone-dependent cancers (adenocarcinoma, prostate cancer, cervix carcinoma, colon cancer, etc.). 1H NMR, 13C NMR and high-resolution time-of-flight mass spectrometry (MS) techniques confirmed the intact structure of the derivative A following its entrapment within HAp/Ch-PLGA particles. The synthesized particles of A-loaded HAp/Ch-PLGA were found to be spherical in shape with a uniform size distribution of $d_{50}$=168 nm. The release of A from HAp/Ch-PLGA was sustained, with no burst release or plateauing after three weeks. The obtained results of the DET and MTT tests show that the particles of A-loaded HAp/Ch-PLGA exhibit almost three times higher cytotoxicity towards lung adenocarcinoma cells (A549) than towards healthy cells (MRC5), while at the same time allowing twice as fast recovery of healthy cells. We have also analyzed the period of recovery of healthy, as well as cancer cells, following the treatment with A-loaded HAp/Ch-PLGA. After treatment with A-loaded HAp/Ch-PLGA, healthy cells recover twice as fast as the malignant ones. Immunofluorescent staining of primary fibroblasts interacting with HAp/Ch-PLGA and A-HAp/Ch-PLGA particles demonstrates no negative morphological or proliferative effects on cells.

O.S.E.3.

# One pot and two step synthesis of 1D and 2D calcium phosphates and their biomedical characteristics

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Calcium phosphate compounds are widely used in bone tissue reparation, engineering, and lately as component of composite drug carriers and sensors. One of the most used methods for synthesis of designed calcium phosphate nanostructures, such as nanowires and tubes, is hydrothermal method. Two different procedures based on this method were used to synthesize hydroxyapatite nanowires. We performed one pot and two step procedures to successfully produce 1D and 2D calcium phosphate compounds with controlled structural and morphological characteristics. The range of techniques such as electron microscopies, XRD, FTIR and laser diffraction were used to induce the properties and formation mechanism of such nanostructures. Compared with one pot, the two step process via DCP platelets as precursor enables more efficient control over HA particle sizes and uniformity. The synthesized 2D DCP and 1D HA particles demonstrated remarkable biocompatibility and no decrease in viability of osteoblastic MC3T3-E1 cells in 2D culture.

O.S.E.4.

## Alginate hydrogels with silver nanoparticles and honey as potential wound dressings

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Alginate hydrogels are widely used as wound dressings due to excellent biocompatibility and high sorption capacity providing regulation of moisture levels in wounds. In order to extend functionality of these hydrogels some of the approaches include addition of silver as a potent antimicrobial agent or immersion in honey to promote healing. In this work, we have developed alginate hydrogels with incorporated silver nanoparticles (AgNPs) and honey components. AgNPs were produced by two methods: electrochemical synthesis in alginate solutions and chemical reduction in aqueous solutions of honey. The obtained Ag/alginate/honey colloid solutions were extruded into a gelling solution ($Ca(NO_3)_2$ x $4H_2O$) in order to produce sheets, microbeads, and microfibers. The colloid solutions and hydrogels were analyzed for stability, potentials for drying and rehydration, AgNP size and silver content. In addition, the nanocomposite microfibers were evaluated in the treatment of second-degree burns in mice showing enhanced wound healing and reepitelization.

O.S.E.5.

## Novel platforms for designing antimicrobial biomaterials

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With more than 4 million operations that include reconstructed surgical procedures which are annually performed worldwide and a fail of about 2% of them because of the infectious- the problem of post-implantation infectious needs novel and more effective solutions. They should not include neither commercial antibiotics nor non-selective, ROS- generating antibacterial nanoparticles. In that context we are developing novel platforms for designing antimicrobial property in biomaterials capable to join effective antimicrobial activity with selectivity in action with bacterial cells. Using natural-sourced molecules (charged amino acids and antimicrobial peptides) conjugated to Au nanoparticles we created enhanced transports to bacterial cells. Alternatively, we designed new antimicrobial nanoparticles (based on Ga and MgO nanomaterials) which use non-ROS mechanisms. In both cases we reached very effective and selective antimicrobial activity and created a promising strategy to design next generation of antimicrobial implants.

O.S.E.6.

## Coupling vanadate elution control with catalytic properties of $V_2O_5$ in $V_2O_5$/PLGA composite coating

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The implant coating technology is seeking for innovative multifunctional materials. They should be able to hinder bacterial growth and stimulate cell attachment on the implant surface. $V_2O_5$ mimics myeloperoxidase activity. This enzyme is located in neutrophils and is carrying out their antimicrobial activity. Further, vanadate ions are formed by $V_2O_5$ dissolution in aqueous solutions. These ions are bioactive at low concentrations.

The described properties of $V_2O_5$ could be exploited for a design of an implant coating, which would exhibit:

- Antibacterial properties, via catalytic action of $V_2O_5$;
- Bioactive properties, via proliferative action of vanadate ions.

$V_2O_5$ is rather soluble in aqueous media at and equilibrium, the obtained amount of vanadate ions is toxic. In order to avoid uncontrolled release of vanadate ions, we embedded $V_2O_5$ nanowires inside poly(lactide-co-glucilode) acid (PLGA) matrix. In this contribution, $V_2O_5$/PLGA ability to i) couple vanadate elution control and ii) catalyse peroxide-to-hypohalite transformation will be discussed.

O.S.E.7.

## Quantifying the fractal dimension and the effective permeability of membrane fouling

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Little is known about the structure of membrane fouling during the ultrafiltration of surface water. A serie of ultrafiltration tests was conducted using feed waters with different combinations of natural organic matter and silica nanoparticles. The goals of the research were: To quantify the fractal structure and the porosity of membrane deposits (Dd and ε) and to identify a correlation between Maxwell model and the permeability of deposits during different stages of filtration. A novel mathematical approach was used to estimate the Dd of growing membrane deposits. A broad range of Dfloc values (1.7 to 2.3) maps onto a narrow range of Dd values (from 2.95 to 3.15), scenario that pointed the importance of breakup and restructuring that aggregates undergo as they are incorporated into a growing cake. Maxwell and Kozeny – Carman models were used to estimate the effective permeability and ε. An hypothesis on aggregate break up and restructuring was set forth.

(*) Current affiliation and sponsorship to attend the conference: Department of Genomes and Supramolecular Chemistry (GEAS), Universidad Regional Amazónica (IKIAM), Vía a Muyuna km 7, Tena, Ecuador. Tel. + 593–6–3700040.

O.S.E.8.

# Effect of cooling rate from α+β range on stereological parameters of microstructure in the $Ti_6Al_7Nb$ alloy

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In the present study the effect of cooling rate from α+β range in the Ti6Al7Nb alloy on microstructure morphology and their stereological parameters is presented. The temperature of heat treatment was selected based on dilatometric and metallographic investigations. The specimens made from $Ti_6Al_7Nb$ alloy were cooled at the different rates, ie. 25, 5, 1 and 0.5°C/s from temperature slightly below the β transus (α+β range) in a high resolution dilatometer. In order to qualitative and quantitative analysis of alloy microstructures, procedures including Thresholding technique and manual stereological measurements were applied. The observed changes in the microstructure were additionally verified by Vickers hardness measurements. The research show that change in cooling rate in range between 25 and 0.5°C/s significantly affects on α and β phase volume fraction as well as their morphology. It was found that the hardness of the $Ti_6Al_7Nb$ alloy is significantly reduced when the cooling rate is less than 5°C/s, which is a consequence of a clear reduction in the volume fraction of β phase. The hardness of the investigated alloy for cooling rate at the 25°C/s is 304 HV10, while for 0.5°C/s is 261 HV10. The research results are relevant to design the heat treatment technology of the alloy and to control its properties.

Acknowledgement: This work has been supported by the National Centre for Research and Development under grant "Heavy-duty friction nodes for biomedical applications”, PBS3/A5/44/2015.

O.S.B.1.

# Boson peak and glass forming ability in CuHfTi metallic glasses

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Unlike many metallic glasses, CuHfTi system for some concentrations can form bulk metallic glass. In order to establish possible correlation between glass forming ability (GFA) and thermodynamic parameters we have measured heat capacity (Cp) for $Cu_{55}Hf_{45-x}Ti_x$ (x=0,5,10, ..., 45) system ranging from 1.8 K up to room temperature for as-cast and annealed samples. Cp of metallic glasses in general does not obey known phonon T3 law which predicts Debye model and one of the anomalies is a wide peak around 10 K which is known as boson peak (BP). Here, we present low-temperature Cp parameters and the intensity of the BP given as subtraction of the measured heat capacity and sum of the Debye phonon and electronic contribution as a function of x. The intensity of BP correlates well with GFA of studied CuHfTi alloys.

O.S.B.2.

# The influence of thermal treatment on physicochemical properties of graphene oxide/phosphotungstic acid nanocomposite

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Graphene and graphene oxide (GO) supercapacitors have attracted considerable attention as novel carbon-based energy storage systems. Because of exceptionally high surface area, lower cost and higher capacitance (compared to graphene), graphene oxide is an ideal support which offers the possibility of integration with different functional materials. In this work, we have investigated the effect of thermal treatment on physicochemical properties of graphene oxide/phosphotungstic acid (WPA) nanocomposite. The nanocomposite has been treated in argon atmosphere and air up to 800 °C and characterized by Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy, X-ray photoelectron spectrometry (XPS), temperature programmed desorption (TPD) and cyclic voltammetry. The multipoint Raman mapping confirmed the homogeneity of the samples, whereas the FTIR analysis showed thermal activation of structural changes of WPA that are atmosphere-dependent. In the case of GO the FTIR analysis showed reduction of intensity of characteristic vibrations of oxygen-containing functional groups with temperature increase. The electrochemical properties of the GO/WPA composite were improved in comparison to pristine GO. In our study, it was showed that the highest increase of both capacitance and operating voltage was achieved at 500 °C. The results suggest that optimization of annealing temperature and GO/WPA ratio are an effective pathway for preparation of hybrid supercapacitors with enhanced properties.

O.S.B.3.

# Influence of point defects concentration on optical and photocatalytic properties of ZnO ceramics

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Zinc oxide is one of the most studied materials due to its wide bandgap (3.37 eV) and large exciton binding energy (60 meV) which enables application in electronics, optoelectronics and spintronics. In the forms of single crystal and thin-film ZnO are used as UV and blue light emitter, while sintered ZnO-based ceramics are important as varistors, thermistors or semiconductors. It has been found that point defects in the crystal structure of a ZnO strongly influenced its electrical and optical properties. Neutral oxygen vacancies are considered to be a major component of the defect structure of ZnO. Thus, correlation of the oxygen vacancies concentration with band gap energy of ZnO product is important to its application in opto-electronic devices.

In this study we investigated the influence of point defects concentration in ZnO crystal structure on its optical and photocatalytic properties. We analyzed ZnO powders prepared by different techniques: (a) microwave processing of precipitate and (b) hydrothermal processing, which yield different ordered crystal structure. To increase a concentration of the point defects in the crystal structure, the powders were sintered in air atmosphere by heating rate of 10 °/min up to 1100 °C, with dwell time of 1 h. The crystal structure, average crystallite size and phase purity of the ZnO ceramics were determined by X-ray diffraction and Raman spectroscopy. The optical properties, in particular, absorption capacity and bang gap energy, were studied using UV–Vis diffuse reflectance spectroscopy. To reveal the role of microstructures and point defects in ZnO crystal lattice, which are receptive for luminescence and photocatalytic activity of this functional oxide, photoluminescence (PL), photoluminescence excitation (PLE) and EPR spectra were analyzed. The influence of point defects concentration in the ZnO crystal structure on photocatalytic properties was examined via decolorization of methylene blue under direct sunlight irradiation. Correlation between amount of the point defects, absorption capacity and photocatalytic efficiency were established. In order to clarify the experimental results ab initio calculations based on density functional theory (DFT) were performed

O.S.B.4.

## Activated track etched carbon for supercapacitor electrodes

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A novel self-supporting carbon thin film supercapacitor electrode was developed starting from polyimide (Kapton) foil. In the first step of the electrode synthesis, latent tracks were inscribed in the starting polymer by irradiation with 253 MeV Kr ions. Next, cylindrical channels were formed by selective chemical etching with NaOCl along the ion tracks, creating track etched polymer. With subsequent carbonization and activation of the track etched polymer, activated track etched carbon was produced. A range of samples were obtained by varying the chemical etching time of the irradiated polymer. The influence of the chemical etching time on the electrochemical properties of the supercapacitor electrodes was investigated by cyclic voltammetry and electrochemical impedance spectroscopy.

O.S.B.5.

## The influence of fluorine doping on the structural and the electrical properties of $LiFePO_4$ powder

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Low intrinsic electronic conductivity is the main weakness of $LiFePO_4$ for the use as cathode material in lithium ion batteries. Here is presented an experimental proof of the theoretical prediction that fluorine doping of $LiFePO_4$ can enhance its electrical conductivity. $LiFePO_4$ and fluorine-doped $LiFePO_4$ olivine type, carbon-free powders are synthesized and examined. Crystal structure refinements in the space group Pnma reveal that doping with fluorine ions preserves olivine structure with the reduction of both the lattice parameters and the antisite defect, and an increase of a crystallite size. A small amount of incorporated fluorine enhances electrical conductivity from $4.6 \times 10^{-7}$ $Scm^{-1}$ to $2.3 \times 10^{-6}$ $Scm^{-1}$ and has positive impact on the electrochemical performances. Several spectroscopy techniques (Mössbauer, FTIR, and Raman) disclose differences between two powders and additionally support the findings of both the Rietveld refinement and the conductivity measurements.

O.S.D.1.

# Designing materials from biological oils

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Oils and fats from living organisms and plants are excellent substrates for new chemistries and design of high value sustainable materials. Designing materials must take into account the structure of lipids. Introduction of functional groups into saturated lipids is made by transesterification or transamidation, whereas unsaturated fatty acids or triglycerides are functionalized by oxidation, epoxidation, hydroformylation, metathesis, ozonolysis, thio-ene reactions with mercaptans etc. Direct polymerization of oils gave liquids of different viscosities useful for printing inks, plasticizers for rubber and modifiers for asphalt etc. Thermosetting oil-based polyurethanes were used for polymer concrete of high quality and as matrix resins for fiber-reinforced composites. Thermoplastic polyurethane elastomers were made from hydroxylated fatty acids. Excellent biodegradable shape memory materials were made from oil-based monomers. Direct polymerization of epoxidized oils lead to pure oil-based polyether foams. The largest outlet for oil-based polyols is in flexible and rigid polyurethane foams. Polyacids from vegetable oils were successfully applied as flexibilizing curing agents for epoxy resins.

O.S.D.2.

# Recovery of rare earth elements of bastnasite ores by advanced hydrometallurgical methods

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In this study the direct acidic leaching of Bastnasite concentrate shall be described in details. The influence of different reaction parameters: fraction size, temperature, concentration of hydrochloric acid, and leaching time on leaching efficiency of rare earth elements shall be considered in order to make scale up of this process. Due to their chemical similarity, the REE separation and purification procedure poses one of the most technical challenges. Fractional crystallization, ion-exchange techniques and chromatographic methods are used to separate them in small amounts. In industrial scale separation generally is achieved using solvent extraction. Solvent extraction is a selective separation procedure for isolating and concentrating substances from aqueous solutions with the aid of an immiscible organic solvent. So far, the performed work has resulted in the separation of heavy (HRE), medium (MRE) and light (LRE) rare earths elements, followed by the separation of yttrium from the HRE fraction and Pr-Nd from the LRE fraction. Thorium removal is following a separate flowsheet. The procedure has gained rapidly growing industrial importance and has been widely adopted for the recovery and separation of base metals and REE.  Specific REE compounds (usually oxides) with purities in excess of 99.99% can be produced.

Acknowledgments: The research leading to these results has received funding from the European Community’s Seventh Framework Programme ([FP7/2007-2013]) under grant agreement n°309373. This publication reflects only the author’s view, exempting the Community from any liability”. Project web site: www.eurare.eu.

O.S.D.3.

# Strength and durability of alkali activated slag in a sea water: influence of alkali ion

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This study aims to understand how the type of alkali activator (Na- and K- activator) affect strength of binders based on alkali activated slag (AAS) and its durability in marine environment. The AAS binders were synthesized using the electric arc furnace slag (EAFS). The results have shown that choice of alkali activator influences the both, the strength and durability of AAS binders. Use of Na-activator promotes the hydration of EAFS and lead to the higher quantity of reaction product which is associated with the higher strength of Na-AAS binders at ambient conditions. Moreover, the Na-AAS binder is characterized by the less porous structure in comparison to the K-AAS binder which is accompanied with the lower sorptivity and better durability of Na- AAS binder in sea water.

PL.S.III.1.

## Grain boundary geometry, structural units and segregation in oxides

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Grain boundary (GB) atomic structures are dependent on the GB characters such as misorientation angle and GB planes. In addition, GB structures are also influenced by the segregated dopants and vacancies to form the relaxed structural units along the GBs. It is therefore needed to investigate the sites of vacancies and dopants segregated at GB, depending on the GB characters, to fully understand GB atomic structures, which are related to the material's properties. In this study, various types of GBs were systematically fabricated for doped and pristine $ZrO_2$, ZnO, $CeO_2$ by the bicrystal techniques, and the structures were characterized with an atomic scale by aberration-corrected STEM, EELS and EDS. Based on the experimental results, the role of segregated dopants and vacancies to change the GB structures were investigated by first principles calculation.

PL.S.III.2.

## Interfacial step alignment as a mechanism of hetero-epitaxy/orientation relationships: the case of Ag on Ni

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How and why do two fcc metals, of very different lattice parameters, choose their relative orientations across their hetero-interface?

To answer this question, the orientation relationships (ORs) of submicron Ag crystals equilibrated on more than 200 Ni(hkl) surfaces, spanning the whole stereographic triangle, have been determined by EBSD. The observed ORs do not conform entirely to either of the common beliefs: (i) that Ag will form with its (111) plane parallel to any Ni(hkl) surface, or (ii) that the OR between Ag and Ni will be cube-on-cube. Although the cube-on-cube OR is indeed observed, three other types of OR have been identified.

The experimental results are consistent with MD simulations, which show that the ORs are related to the step alignment which develops in the early stages of interface formation and which leads to minimum energy interfaces. This is a new concept for the interpretation of hetero-epitaxy and/or ORs.

PL.S.III.3.

## Controlling Microstructural Evolution via Adsorption

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The role of dopants in processing ceramics has been an important issue for many years, especially given the contradicting reports of retarded or accelerated grain growth by key dopants and impurities. We have developed a technique to experimentally measure dopant solubility limits at the sintering temperature, such that actual dopant levels can be associated with equilibrium grain boundary (GB) segregation (below the solubility limit) or with enrichment (above the solubility limit). New analysis of GB mobility of alumina as a function of dopant concentration has shown that some segregating dopants increase the GB mobility, i.e. the opposite of solute-drag. The segregating dopants are associated with 2-D structural and compositional (complexion) transitions at the GBs, and possible changes in the mechanism of GB migration. This presentation will review recent GB mobility measurements and the concept of 2-D GB transitions, and their potential use for controlling the microstructural evolution of polycrystalline ceramics.

PL.S.III.4.

## TEM observation of atomic structures and their evolutions in 2D and 1D materials

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Properties of low-dimensional material highly depend on its atomic structure. The studies of atomic defects and boundaries are of general interest for the fundamental researches and technological applications in any crystalline materials, especially in 2D materials. Point defects and edge structures of graphene have been intensively studied with atomic precision in the last decade. Here I present some new examples for atomic-scale imaging and spectroscopy of various low-dimensional materials with interrupted periodicities. Nitrogen defects and their chemical dynamics of graphene are now studied at individual atom basis [1]. Defects and phase transitions of single-layered dichalcogenides (MX2) are corroborated in situ [2]. In plane anisotropy of single-layered group VII dichalcogenides ($ReS_2$ and $ReSe_2$) is recently reported [3]. Also various new 1D structures inside carbon nanotubes are discovered and investigated [4, 5, 6]. Eventually single atom magnet at grapheme atomic defects will be proposed [7].

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PL.S.III.5.

## Atomic Structure of defects, dopants and edge terminations in monolayer 2D materials

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Defects and dopants in 2D materials influence their properties and understanding their structure at the atomic level is crucial. I will show how aberration corrected transmission electron microscopy is used to probe graphene and $MoS_2$ monolayers at the atomic level. This will include vacancy defects, substitutional dopants and surface adatoms. Combining scanning transmission electron microscopy with electron energy loss spectroscopy enables single atom measurements of bonding states and elemental identification. Using an in-situ heating holder, I will show how the migration of vacancies leads to new defect structures not seen at room temperature. Edge terminations are also shown, presenting low energy reconstructions that help minimize strain and unsaturated bonds.

PL.S.III.6.

## Atomic collapse in graphene

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The chiral nature of charge carriers in graphene prohibits backscattering and prevents confinement by electrostatic potentials, resulting in high electronic mobility and unusual phenomena such as Klein tunneling. This picture breaks down in the presence of charge impurities exceeding a critical value $Z_c$, where a qualitative change in behavior leads to the capture of electrons akin to atomic collapse in 3D atoms. Although in graphene $Z_c$ is substantially lower than in 3D atoms, attaining the supercritical regime is difficult because screening can significantly reduce the effective charge of the impurity.

The transition from sub-critical to the supercritical regime is accompanied by trapping of electrons in quasi-bound states which are the condensed matter analogue of the long sought after phenomenon of atomic collapse in super-heavy nuclei. The quasi-bound electron-states show up as a strong enhancement of the density of states within a disc centered on the vacancy site. We find that these states are surrounded by a circular halo of hole states which are interpreted as the analogue of positron production in atomic collapse. We further show that the quasi-bound states at the vacancy site are gate tunable and that the trapping mechanism can be turned on and off, providing a new paradigm to confine, control and guide electrons in graphene.

PL.S.III.7.

# Aberration corrected views of of chemical ordering and segregation in complex oxides

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The properties of complex oxides are extremely sensitive to minor changes in doping. For example, in manganites it is still not clear whether chemical order (or disorder) is in any way connected to phenomena such as double exchange, electronic phase separation or charge ordering. By means of aberration corrected scanning transmission electron microscopy (STEM) and electron energy-loss spectroscopy (EELS) combined with simulations it is possible to carry out atomic resolution studies of these systems, such as the colossal magnetoresistant manganite $La_{2-2x}Sr_{1+2x}Mn_2O_7$ [1-3]. For this material we find a significant degree of long-range chemical ordering for a number of values of doping (x), which increases in the antiferromagnet- charge ordered range. However, the degree of ordering is never complete. Our results show that chemical ordering over distinct crystallographic sites is not needed for electronic ordering phenomena to appear in manganites, and other explanations, including electronic degrees of freedom, play a determining role when trying to explain the complex electronic behavior of manganite oxides. In fact, STEM-EELS studies of this type provide the key to harness other oxide systems where minor changes in local composition may have a direct effect on macroscopic properties. An example can be found in ionic conductors such as those in polycrystalline solid electrolytes. They are the main component in solid-state electrochemical devices, such as fuel cells and batteries but their performance is strongly limited by ion blocking at grain boundaries in the electrolytes. Understanding the chemical, structural and electronic properties of these materials at the atomic scale is the key to improve functional properties and the door to designing low power energy generation and storage devices [4,5]. Here, we will discuss a STEM-EELS study of a single grain boundary in a bicrystal of yttria (9% mol) stabilized zirconia, an emblematic oxide ionic conductor. From strain analysis and atomic resolution EEL spectrum images, we find a strong tendency to yttrium segregation at the expansive site of the grain boundary cores, doubling the bulk relative Y concentration. Contrary to previous reports [6], we detect a depletion of oxygen within a region of nanometric dimensions around the boundary, which may be explained by the presence of O vacancies [7]. We will discuss these findings in the light of density-functional theory calculations.

Acknowledgements: Work done in collaboration with Gabriel Sanchez-Santolino, J. Salafranca, M. A. Frechero, M. Rocci, Rainer Schmidt, M. R. Díaz-Guillén, O. J. Durá, A. Rivera-Calzada, R. Mishra, M. A. Roldan, M. P. Oxley, Q. A. Li, H. Zheng, K. E. Gray, J. F. Mitchell, Carlos Leon, S. T. Pantelides, Jacobo Santamaría and Stephen J. Pennycook. Research at UCM sponsored by Fundación BBVA and Spanish MINECO MAT2015-66888-C3-3-R. Research at Oak Ridge National Laboratory supported by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division, and through a user project supported by ORNL's Shared Research Equipment (ShaRE) User Program, which is also sponsored by DOE-BES.

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PL.S.IV.1.

# Towards device physics of the $CH_3NH_3PbI_3$ photovoltaic perovskite

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Recently, it has been shown by the Snaith[1] and Graetzel[2] groups that $CH_3NH_3PbI_3$ is very promising material in photovoltaic devices reaching light conversion efficiency (η) up to 21%. A strong research activity has been focused on the chemistry of the material to establish the most important parameters which could further improve η and to collect photons from a broad energy window. The major trend in this field is in photovoltaic device engineering although the fundamental aspects of the material are not yet understood.

In my lab we have devoted considerable effort to the growth of high quality single crystals at different length scales, ranging from large bulk crystals (up to 100 $mm^3$) through nanowires[3,4] down to quantum dots of tens of nanometers of linear dimensions. The structural tunability of the material allows to study a broad range of physical phenomena including electrical and thermal transport, magnetism and optical properties which will be reported in this presentation together with some device applications[5].

Acknowledgement: The work has been performed in collaboration with Endre Horvath, Massimo Spina, Balint Nafradi, Alla Araktcheva, Andrea Pisoni, Jacim Jacimovic and the Van der Marel group. This work was partially supported by the ERC Advanced Grant (PICOPROP#670918).

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PL.S.IV.2.

# Tailoring defined-shape ferroelectric particles for various ferro- and piezoelectric applications

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Ferroelectric perovskites exhibit great potential for many applications that require a size down to the nanometre range. For this reason the interest in preparing defined-shape ferroelectric nanoparticles has increased tremendously in the past 10 years. These ferroelectric nanoparticles, with a unique anisotropic shape and size-dependent properties that differ from their bulk counterparts, also represent a challenge to fabricate the nanostructures via their self-assembly. If the direction of spontaneous electric polarization of the ferroelectric particles could be tuned, then these particles or their self-assembled structures are expected to make a significant breakthrough in the field of memory storage, piezoelectric sensors, ferroelectric-photovoltaic devices, photocatalysis and energy harvesting.

Due to the high symmetry of their crystal structure, $ABO_3$ perovskites do not show a tendency to grow in defined anisotropic shapes such as plates or needles. In this presentation a critical overview of past research will be presented. In addition, a study of the formation and the resulting properties of perovskite $Ba_{1-x}Sr_xTiO_3$ micro- and nano-plates that were realized by the *in-situ* topochemical transformation of the layered perovskite $Bi_4Ti_3O_{12}$ precursor template will be reported. The influence of the $Bi_4Ti_3O_{12}$ template dimensions, the Ba/Sr ratio and the conversion conditions on the size, tetragonality and orientation of the single-crystalline $Ba_{1-x}Sr_xTiO_3$ micro and nano-plates were also examined in great detail. The main focus was on preparing highly tetragonal (002)-oriented $Ba_{1-x}Sr_xTiO_3$ plates with nano dimensions. Their piezoelectric, ferroelectric characteristics and domain structure were studied by means of electron microscopy, differential scanning calorimetry (DSC) and piezo-force microscopy (PFM).

For these materials, the application potential of highly oriented, micro- and nano-plates based on $Ba_{1-x}Sr_xTiO_3$ will be discussed.

PL.S.IV.3.

## How could electrolytes and electrodes be friendlier for Li-ion traffic?

Mamoru Senna
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During charging and discharging of lithium ion battery (LIB), Li-ions are always forced to move downwards or upwards as quickly as possible. This is particularly important, when we are dealing with all-solid LIB. For one of the most promising solid state electrolytes, garnet type cubic $Li_7La_3Zr_2O_{12}$ (c-LLZO), efforts were paid to increase their ionic conductivity, mainly by replacing some of the cationic species, instead of improving their solid state preparative processes (SSPP). Similar is true for anode materials, e.g. spinel $Li_4Ti_5O_{12}$ (LTO). SSPP will improve the Li-ion traffic throughout LIB.

The present talk starts with solid state processes for c-LLZO and LTO at lowest possible temperature to suppress their grain growth. Their electrochemical behaviors in conjunction with their overall Li-ion battery properties are then discussed. Emphasis is laid on the relationship between the chemical and structural states of c-LLZO and LTO and their overall electrochemical performances in some prototypic LIB.

PL.S.IV.4.

## Recent progress in R&D of the primary particles of detonation nanodiamond

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The latest results from our laboratories on the R&D activities of the primary particles of detonation diamond (PPDND) will be briefly introduced, which include determination of an average diameter of PPDND to be 2.8(5)nm and geometrical as well as electronic structure of unique core-shell composition. Three major applications that are being developed by us including nanospacer lubricants, nano-composites and drug carrier for cancer chemotherapy will be mentioned in some detail. PPDND appears to be a prototype of nanocarbons like $C_{60}$ and CNT appeared recently and under active exploitation.

PL.S.IV.5.

## Nanodiamond and its derivatives for catalysis

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Nanodiamonds (ND) are commercially available by detonation of explosives under oxygen-deficient conditions. The structure of these particles is a crystalline sp2 -bonded diamond core, surrounded by few layers of disordered $sp^2$ /$sp^3$ carbon, resulting in a variety of oxygen terminations on dangling bonds and defects on surface. The chemical nature of ND surface can be tailored by the surface sp /sp hybridization state, defect and decoration with various heteroatom functionalities. We have used surface-modified ND as catalyst and catalyst support for heterogeneous catalytic reactions that show unusual performance. For oxidative dehydrogenation of n-butane, the ND exhibited superior performance than other nanocarbon materials. ND also showed better performance in direct dehydrogenation of ethyl benzene to styrene; Nitrogen and boron doped annealed ND is also electro-active for ORR, but the performance is still needed to be optimized. The state-of-the-art of ND catalysis will be presented with an outlook for practical application.

PL.S.IV.6.

## Scaffolds for tissue repair and regeneration

Serena Best
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Advances in regenerative medicine are dependent on the development of scaffold materials which offer a bioactive, three dimensional environment for the support of cells and new tissue. Key to the development of these scaffolds is an understanding of their physical, chemical, mechanical and biological properties to ensure optimised clinical performance. We have established a range of methods for the production of scaffolds based on collagen and also calcium phosphates (and in particular, synthetic hydroxyapatite ($Ca_{10}(PO_4)_6(OH)_2$). While the control of structure and chemistry over a range of length-scales is reported widely, there are a number of areas which are still relatively poorly understood. This talk will provide insights into the effects of collagen-based structures produced via freeze-drying followed by zero length cross linking to produce 3D collagen environments for tissue regeneration. In any scaffold, pore size and orientation are crucial in their design, to provide appropriate three dimensional pore structures, however we have also shown that the percolation diameter is a key parameter with a threshold value below which significant invasion is not seen. We have also developed improved understanding of the effects of selective attachment of peptide sequences to scaffold surfaces to illicit specific cell signalling and intergrin binding. It is through this work, providing deeper understanding of the processing and properties of scaffolds, that the clinical success of implants will be assured.

PL.S.IV.7.

# Advanced and in situ transmission electron microscopy of semiconductor nanowire materials

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Advanced high-resolution imaging and spectroscopic techniques of transmission electron microscopy (TEM) play a crucial role in characterizing the structure-property relationships of inorganic functional materials and interfaces. The microstructure, the elemental composition, and the physical properties of nanomaterials can be characterized quantitatively and with spatial resolutions in the nanometer regime or even on the atomic level. This report describes two applications of in situ studies to semiconductor nanowire (NW) materials.

The first example illustrates phenomena that occur under thermal load of ZnO NWs (dimensions $\leq$ 100nm) with core materials of low melting temperature [1-3]. ZnO NWs fabricated by thermal methods from Sn-based precursor materials under certain conditions possess nanotube-like core-shell morphologies with partially or completely filled core regions. Scanning transmission electron microscopy (STEM) combined with energy-dispersive x-ray spectroscopy (EDXS) confirm the presence of a Sn or a Sn-rich core material [2]. When exposing the NWs alternatingly to high and low electron beam fluxes, melting, re-solidification, and the reversible thermal expansion and contraction of the molten core material can be observed by in situ TEM. These methods enable monitoring the behaviour of the core and the modification of its chemical composition during extended thermal cycling.

The second example illustrates the effects of elastic straining on electronic and on electrical transport properties of individual GaAs and InAs semiconductor NWs (diameters $\approx$ 100nm, lengths $\geq 5\ \mu$m) [4]. Using a TEM holder equipped with a piezo-controlled scanning tunnelling tip [5] allows the application of controlled values of elastic strain to individual NWs while simultaneously monitoring their electronic properties by valence electron energy loss spectroscopy (VEELS), measuring their change in electrical resistance by taking I-V curves, and imaging their morphology and microstructure. Elastic bending experiments reveal that the GaAs NWs are highly flexible. I-V plots show an increasingly non-linear behavior with increasing strain. NW morphology and the electrical properties are restored upon complete strain release. The VEELS measurements show changes of the electronic band structure with bending for the GaAs and the InAs NWs. The impact of strain and other possible influences on the electronic and transport properties will be discussed.

It is my pleasure to acknowledge the collaborations with my colleagues and co-authors mentioned in the references.

1. Authors: Yanicet Ortega[a,b], Dietrich Häussler[a], Paloma Fernández[b], Javier Piqueras[b], and Wolfgang Jaeger[a] ([a]Institute for Materials Science, Christian-Albrechts-Universität zu Kiel, Kiel, Germany, [b]Dept. Materials Physics, University Complutense of Madrid, Madrid, Spain)
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PL.S.V.1.

## Neutron scattering and atomistic modeling for materials science

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Neutron scattering has long history of application in materials science. High penetrating power of centimeter size neutron beams allows to study bulk samples often in situ or in operando under conditions similar to real life environment. In parallel, the recent past has seen rapid development of methods and codes for classical and ab initio calculations which can now accurately model crystal structure and dynamics of materials at the atomic scale. I will present recent examples of complementing neutron scattering experiments at ANSTO with atomistic modeling that led to new insights into relationships between structure and physical properties of interest in various advanced materials of technological importance.

PL.S.V.2.

## Understanding failure and fatigue mechanisms of advanced and natural polymer fibres by Raman/IR microspectrometry

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A very important characteristic of the mechanical properties is that they do not only depend from the matter, but also from the object: in a rough description, as a function of the 'quality' of the sample processing, it is more or less possible to explore the potential of the mechanical properties of the material. We will review the broad possibilities that Raman – and some extended IR-microspectrometry in combination with tensile/compressive solicitations offer in the study of the (nano)texture and the (nano)mechanical behaviour of advanced and natural fibres by closely analysing the spectra in two wavenumber ranges that are generally ignored in polymer materials studies, the very low (< 200 $cm^{-1}$) and the very high ( ~3500 $cm^{-1}$) wavenumber ranges. Techniques of deuteration developed for the study of protonic conductors will be also dealt with. We will consider the most important synthetic (polyamides (PA 66), polyethyleneterephthalate (PET), polypropylene (PP), poly(paraphenylene benzobisoxazole (PBO), Kevlar) and natural (keratin/hair, silkworm and spider silks) fibres. Vibrational spectroscopy is applied so as to differentiate between crystalline and amorphous macromolecules. These conclusions are then used to discuss the modifications induced by the application of a tensile or compressive stress, including the effects of fatigue. Detailed attention is paid to the inter-chain coupling for which the importance of hydrogen bonding is reconsidered. The significant role of the ‘‘amorphous’’ bonds/domains in the process of fracture/fatigue is shown.

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PL.S.V.3.

# High-melting point compounds: new approaches and results

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New subjects in the field of high-melting point compounds, such as MAX-phases (where M is an early transition metals, A is an A-group (12-16) element, and X is carbon/nitrogen), MXenes (graphene analogues), 2D BN nanosheets, high-entropy nitrides/carbides, and twinned structures, are described in details. New experimental and theoretical results are discussed and compared with those for traditional carbides and nitrides. Special attention is paid to the new nanomaterials stability under thermal, irradiation, deformation, and corrosion actions. New spheres of possible applications are highlighted. Some unresolved problems are emphasized.

PL.S.V.4.

# Deformation Mechanisms, Microstructure, and Mechanical Properties of High-Mn Austenitic Steels

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A new class of austenitic steels stabilized with high-Mn contents (instead of Ni) exhibits exceptional mechanical properties, such as large energy absorption and high work-hardening rate, owing to secondary deformation mechanisms such as mechanical twinning-induced plasticity (TWIP) and martensitic transformation-induced plasticity (TRIP) favored for low stacking-fault energy (SFE) [1]. The interaction of dislocations with twin boundaries and martensite interfaces during mechanical deformation enhances the work hardening, i.e., a dynamic Hall-Petch effect, with total elongations exceeding 70% and ultimate tensile strengths in the GPa regime. The influence of the strain rate, temperature, and changes in SFE on the deformation mechanisms in high-Mn austenitic steels has been investigated using electron backscattered diffraction (EBSD), electron-channeling contrast imaging (ECCI), conventional bright-field/dark-field imaging (BF/DF), and aberration-corrected high-resolution transmission electron microscopy (HRTEM). The TWIP/TRIP secondary deformation mechanisms are related to the low SFE exhibited in these materials. Experimentally measured SFE from weak-beam-dark-field (WBDF) imaging provides the basis to understand how changes in SFE influence mechanical twinning versus transformation induced martensite [2-3]. However, adiabatic heating during deformation at high strain rates (100 -10,000 s-1) increases the SFE. Quantifying the twin or martensite density by EBSD/ECCI and BF-DF images allows for comparison of the secondary deformation at different SFE, strain rates, and total elongation, but to study the details of the deformation mechanisms requires imaging at atomic resolution using aberration corrected HRTEM. This presentation will correlate the mechanical properties of high-Mn austenitic steel with the deformation mechanisms and microstructure for strain rates from $10^{-4}$ to 103 $s^{-1}$.

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PL.S.V.5.

# Hyaluronate-based thermo-sensitive hydrogel as cell carrier for nucleus pulposus regeneration and vitreous body substitute

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Intervertebral disc degeneration usually starts at the nucleus pulposus. In the past decades, several techniques and prosthetics (artificial disc) have been developed to regenerate or replace the nucleus pulposus. However, these kind of pre-formed devices have to remove the nucleus pulposus and then replace an artificial one to relief the symptom of intervertebral disc degeneration. Recently, cell-based tissue engineering provides a rational approach to regenerate active nucleus pulposus cells (NP cells) to restore intervertebral disc architecture and function. However, the source of autologous nucleus pulposus cells are limited and their functional state does not favor regeneration. Besides, nucleus pulposus cells grown in monolayer may result in fibroblast-like transformation. Thus, the 3D hydrogel co-culture system maybe an alternative method to provide an adequate environment for nucleus pulposus cells proliferation, extracellular matrix production, cytokines secretion.

Human vitreous is a gelatinous substance that is predominantly composed of collagen fibril, hyaluronic acid (HA) and water (97–99%). Vitreous substitutes are needed to tamponade the detached retina after vitrectomy when treating retinal detachments. However, several drawbacks associated with current vitreous substitutes have been reported. In the present study, we developed a colorless, transparent and injectable hydrogel as a vitreous substitute that was formed by oxidated HA (oxi-HA) and adipic acid dihydrazide (ADH). The results of biodegradation demonstrated that the hydrogel could maintain its gel matrix over at least 35 days depending on the ADH concentration. In addition, the biocompatibility was evaluated on a retina pigmented epithelium (RPE) cell culture following ISO 10993-5 (tests for in vitro cytotoxicity), and the hydrogel was found to be nontoxic. This study suggested that the injectable oxi-HA/ADH hydrogel could fulfill many critical elements that are desirable in vitreous substitutes.

PL.S.V.6.

## From controlled drug delivery to gene therapies to bone regeneration: calcium phosphate nanoparticles as essential components of advanced biomaterials

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Calcium phosphate is the most natural inorganic substitute of boney tissues. Yet, because of its ordinariness and specific weaknesses – e.g., low capacity for stable conjugation with active compounds, weak morphological control and a large propensity for aggregation - it has frequently been denounced as a material of the past. Its use is currently on the way to be reduced to the strengthening and osteoconductive component of tissue engineering constructs only. However, the structural complexity of calcium phosphates is immense and, especially in the nanoparticulate form, they are able to display an array of exciting properties that go beyond those for which they have been standardly known. These properties will be elaborated in this lecture and include the ability to achieve sustained and tunable drug release profiles; injectability; the osteogenic potential and the ability to inhibit osteoclastogenesis; usability for the intracellular delivery of bioactive compounds; antimicrobial activity; and processability into macroporous tissue engineering constructs. A precise design of materials based on calcium phosphate nanoparticles only is expected to lead to a new generation of materials for therapeutic and regenerative purposes. Such materials would make the use of expensive bone growth factors, antibiotics, viral vectors and polymers as viscous components unnecessary. They would be classifiable as socially aware materials due to their applicative elegancy, inexpensiveness, in situ synthesizability and easy transferability across the rich-poor gap.

# Poster Presentation

P.S.A.1.

## Novel pathway towards the synthesis of complex double perovskites

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The simultaneous presence of ferromagnetism and ferroelectricity in a single phase and possible spin-phonon couplings in these systems offers the appealing opportunity to design unconventional devices, such as multiple-state memory elements and electric-field controlled magnetic sensors. Mixed double perovskites, due to its structural diversity, represent a very promising platform in a quest for new multiferroics. A new synthesis route for the preparation of mixed metal oxides crystallizing in the double perovskite structural type will be presented and discussed. This procedure includes the thermal decomposition of the mixture containing two heterometallic molecular precursors (Ba-Nb oxalate- and Ni-Ta oxalate-based complexes!), in a specific ratio. A detailed X-rays powder diffraction study has been carried out in order to examine structural features of prepared oxide material containing two metals on both crystallographic sites (A and B) within perovskite lattice. The effect of thermal decomposition temperature on the microstructural parameters will be discussed as well.

P.S.A.2.

## High-temperature treatment for new properties of $LuPO_4$:Eu, $Lu_2O_3$:Tb,Ti/Hf and $BaHfO_3$:Pr

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$Lu_2O_3$, $LuPO_4$ and $BaHfO_3$ are heavy compositions and thus attractive hosts for scintillator materials. Yet, the orthophosphate cannot be made as large single crystals, lutetia does not allow for fast Ce or Pr emissions and the hafnate produce only moderate scintillation when doped with Ce. These problems precluded broader applications of luminescent materials based on the three hosts till now. However, we shall show that all the three compositions produce efficient thermoluminescence (TL) when activated with selected lanthanides and fabricated in specific conditions.

The presentation will focus on revealing how deeply the spectroscopic properties of the title composition are affected by the high-temperature treatment. The advantages of the TL properties of the discussed materials over those already known will also be considered.

Acknowledgements: Financial support by the Polish National Science Centre (NCN) under the grant #UMO-2014/13/B/ST5/01535 ($Lu_2O_3$:Tb,Ti/Hf), and by EU under the Marie Curie Initial Training Networks (ITN) action, LUMINET project, grant No. 316906 ($BaHfO_3$:Pr) as well as from Krajowy Naukowy Osrodek Wiodacy (KNOW) through Wroclawskie Centrum Biotechnologii is acknowledged (LuPO4:Eu).

P.S.A.3.

## Processing and characterization of dental acrylate improved with zirconia

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Poly (methyl methacrylate) (PMMA) is one of the polymers commonly used in dentistry as it shows good biocompatibility and has the possibility to withstand the conditions required. Zirconia is one of the oxides used to improve thetmal, mechanical and optical properties of the polymer matrix in dental composites. Zirconia is inert in contact with the organism and is possible to obtain in different forms of particles. Processing and characterization of PMMA-$ZrO_2$ dental composites is presented in this study. The specimens were prepared in aluminium mold with thermally polymerized acrylate with different content of zirconia. FTIR analysis performed to investigate bonding between zirconia and matrix. Thermal properties of composite were analyzed by DSC. Mechanical charaterization of samples were performed. Low energy impact test was performed in order to determine mechanical properties of composites. The adding of zirconia improved thermal and mechanical properties and resistance to impact compared to the pure polymer.

Acknowledgement: This research was financed by the Ministry of Education, Science and Technological Development of the Republic of Serbia as a part of the project TR34011 and III45019.

P.S.A.4.

## Biocompatible poly(methyl methacrylate)/di-methyl itaconate – (iron oxide dopped alumina) composite with improved mechanical properties

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Poly (methyl methacrylate) (PMMA) copolymerized with di-methyl itaconates exhibits improved biocompatibility for dental use as it loweres the quantity of residual monomer. The aim of this study is to improve mechanical properties decreased with itaconate using iron oxide dopped alumina particles. Submicron particles were synthesized via sol-gel technique. The composites having 1, 3 and 5 wt. % particles were prepared. Polymerization was done using the standard procedure recommended by the supplier. Obtained composites were tested using standard mechanical testing procedures to monitor the behavior under tension and bending. The results were used to obtain the modulus of elasticity. Low energy impact test was used to measure the toughness of specimens. The aim of these procedures was to observe the influence of addition of particles to the polymer matrix and to improve mechanical properties compared to modified PMMA polymer.

Acknowledgement: This research was financed by the Ministry of Education, Science and Technological Development of the Republic of Serbia as a part of the project TR34011.

P.S.A.5.

## Rapid fabrication of antimicrobial poly(vinyl butyral)/ titania nanofibers using multi-needle electrospinning

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Titania nanofillers were used to reinforce nanofibers in composite mats produced via electrospinning of poly(vinyl butyral) (PVB) with two different concentrations of polymers. The (TTNP) titania nanoparticles and (TTNT) titania nanotubes were added into acetic acid/ethanol solution in different contents 3 wt. % and 1 wt. %, respectively. The effect of the processing system on the morphology of the produced fibers was analyzed. The antimicrobial PVB composite fibers with titania nanoparticles and titania nanotubes were produced by single and multi-needle electrospinning system. The results showed that the composite mats with PVB nanofiber incorporating TTNP exhibited similar antibacterial efficiency compared to the mats containing the TTNT nanofiber composites. The results confirmed that the PVB/TTNP nanofibers, as well as the PVB/TTNT nanofibers gave 80% and 163% improvement in indentation hardness together with 61% and 84% improvement in the reduced elastic modulus, respectively, compared to the neat PVB nanofibers (produced from the multi-needle system). In this study, it was important to produce the composite nanofibrous mats with significant mechanical and antimicrobial properties at a high production speed, which is promising for commercial application.

P.S.A.6.

## Thin films of $MoS_2$ on $Cu_2O$ as biosensors

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Layered dichalcogenides of transition metals $MQ_2$ (M = Ti, Nb, Mo, W; Q = S, Se, Te) have been extensively studied for more than three decades, but their electronic nature remain a matter of debate to this day. Remarkable electronic and optical properties of dichalcogenides allow use some of them as photocatalysts, battery cathode materials including solar energy conversion units, optoelectronic sensors etc.

This work is devoted to preparation of thin films of $MoS_2$ on $Cu_2O$ surface and investigation of stability of $MoS_2$ / $Cu_2O$ system at heating. Two methods for preparation of such thin films were studied: a) thermal decomposition of volatile compounds containing Mo and S (MO CVD process); b) spray method using colloidal dispersions of $MoS_2$ in organic solvents. The materials prepared were characterized by different methods.

The work is carried out in the framework of the Russian-Taiwanese joint research project “Nano-heterostructures "Graphene / Metal oxides / metal chalcogenides" for use as a single-cell biosensors with improved photoelectrochemical properties and self-powered”.

P.S.A.7.

## PVA membranes doped with Ti and Zr oxide for alkaline electrolysis with ionic activators

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Separator membranes were prepared from 5 and 10 wt. % solution of polyvinyl alcohol by physical cross-linking during freeze-thawing process, with addition of titanium dioxide and zirconium dioxide in starter solution. Compared with commercial membrane this types of membranes showed same or in some cases even better electrochemical performance at ambient temperature and pressure, but the process of preparation is much easier and cost less. The resulting current density versus voltage showed decreasing voltage with adding ionic activators based on cobalt and molybdenum for about 27 % when used 10% PVA/$ZrO_2$ and 20% with 10% PVA/$TiO_2$. Conductivity measurements by the impedance technique using a two-probe method indicated that 10% PVA/$TiO_2$ have ionic conductivity of about 0.05 $Scm^{-1}$, very similar as commercial membrane. Testing of mechanical properties showed that prepared membranes have maximal stress before breakage from about 12 to 18 MPa which is close to the results of commercial membrane.

The authors would like to thank the Ministry of the Science of the Republic of Serbia for the financial support through Project No. 172045.

P.S.A.8.

## Influence of the nickel loading and the calcination temperature on the activity of NiO-$Al_2O_3$ catalyst prepared by mixing powders of metal oxides in the partial oxidation of methane

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The influence of the nickel content and the calcination temperature on the activity of the NiO-$Al_2O_3$ catalysts was tested in the partial oxidation of methane. The samples with a 5 wt%, 10 wt%, 20 wt% NiO, were prepared by the method of mechanical mixing powders of metal oxide. The catalysts were subsequently heat treated by calcining, respectively at temperatures of 400 ºC, 700 ºC, 1100 ºC. The reaction is carried out in a laboratory test reactor at the Faculty of Technology in Novi Sad. In the catalysts prepared by mechanical mixing, expressed the weak interactions of the active phase and support and consequently, the active phase is more easily released. NiO is randomly distributed on support, being manifested by varying the activity values and the activity is also hard to predict in the test series. The presence of free NiO increases catalyst activity at all tested temperatures calcination and quantities of the active phase; but does not contribute to leveling the value of activity in the test series of samples in the observed reaction conditions.

P.S.A.9.

# Structural and magnetic properties of mechanochemically synthesized $LaFe_{1-x}Cr_xO_3$ (x = 0.5 and 0.75)

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Perovskite oxides with the composition $LaFe_{1-x}Cr_xO_3$ (x = 0.5 and 0.75) have been studied. The samples have been prepared using the mechanochemical treatment. A mixture of crystalline $La(OH)_3$, $Fe_2O_3$ and $Cr_2O_3$ powders in stoichiometric ratio was mechanochemically treated in a planetary ball mill up to 40 h of milling. The mechanochemical formation of the $LaFe_{1-x}Cr_xO_3$ perovskite phase was followed by X-ray diffraction and magnetization measurements. The Rietveld refinement of the XRD data shows that the compounds crystallize in an orthorhombic perovskite structure with a random distribution of the Fe and Cr cations at the B sublattice. All structural and microstructural parameters were analyzed. In addition, magnetic measurements for $LaFe_{0.5}Cr_{0.5}O_3$ show clear antiferromagnetic ordering bellow 250 K, which supports above conclusion of random distribution of Fe and Cr cations.

P.S.A.10.

# Surfactant-assisted high energy ball milling technique as a method for preparation of magnetic submicrometer particles

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Production of $Nd_2Fe_{14}B$ magnets from submicron grain size particles is important task nowadays both from the point of increased coercivity and to eliminate the need for corrodible grain boundary phases. One of the approaches for preparation of magnetic nanoparticles is by application of surfactant-assisted high energy ball milling (SA HEBM) technique. High energy ball milling (HEBM) have been used for mechanical grinding of very coarse-grained HD (Hydrogenated Disproportionated) $Nd_2Fe_{14}B$ particles to micrometer range, but it have been found that this process had inherent limitation and additional grinding did not result in a further reduction of particle size. In an attempt to further reduce the particle size in submicrometer range wet HEB milling was introduced. Wet milling without surfactant is equivalent to dry milling except decreasing the milling efficiency and friction because of the presence of liquid medium. It was shown that presence of surfactant is crucial at impeding cold welding and the agglomeration of particles during ball milling. In this work, we report our results on producing NdFeB particles in sub micrometer range and study their size and properties as a function of the different milling conditions (milling speed and duration, ball to powder ratio, BPR, etc.).

Acknowledgements: This work is funded by FP7 project MAG-DRIVE: "New permanent magnets for electric-vehicle drive applications", grant agreement no: 605348.

P.S.A.11.

# Characterization of NdFeB magnetic submicron particles obtained by surfactant-assisted high energy ball milling (SA-HEBM)

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Research relates to characterization of submicron particles obtained by the comminution of NdFeB magnetic material employing surfactant assisted high energy ball milling (SA HEBM) is given. Milling experiments were carried out in different ways, only SA-HEB milling and successive dry and wet SA-HEB milling. During wet milling a suspension was obtained along with slurry which is sedimented on the bottom of the milling bowl. SEM characterization was performed on non-aligned and magnetically-aligned slurry and suspension. Closely-packed NdFeB submicron particles in slurry and suspension were confirmed. In order to indicate carbon abundance change in the specimen for different milling conditions, EDX analysis was performed and it was shown that successive dry and wet milling operations lead to intensive surfactant adsorption on particles. Mercury Intrusion Porosimetry was used to determine the particle size and the particle size distribution in the slurry, related to pore size and the pore volume distribution. Samples for X-ray Powder Diffraction Analysis were prepared by embedding the slurry in a two-component epoxy resin, without aligning in magnetic field. The presence of expected $Nd_2Fe_{14}B$ crystalline phase was determined.

Acknowledgements: This work is funded by FP7 project MAG-DRIVE: „New permanent magnets for electric-vehicle drive applications“, grant agreement no:605348.

P.S.A.12.

# Experimental and theoretical analysis of fullerenol nanoparticles/water system

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Solubility in water is one of the main requirements concerning bioapplication of fullerenol nanoparticles (FNP), therefore we conducted experimental and theoretical analysis of interactions between FNP and water molecules. According to the obtained results, modifications of fullerene with OH groups led to the substantial improvement of interactions with water for more than five times in comparison to native fullerene molecule. Radial distribution functions (RDF) of fullerenol indicate pronounced interactions of oxygen and hydrogen atoms with water molecules, too. In order to discuss nature of interactions and structuring of water in the investigated fullerenol/water system, we calculated fullerenol's volumetric properties. The results of Masson’s coefficient calculation showed weak solute-solute interactions, and the weakening of the interactions between FNP and water molecules at temperatures higher than 309,15 K. Furthermore, the results also indicated fullerenol structure-making properties.

P.S.A.13.

# Highly efficient graphene supports for fuel cells

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Nanomaterials based on graphene are highly important because of their unique properties for example high contact surface area, high electrical conductivity and their enormous stability. Graphene and graphene related materials have been used as promising catalyst supports in energy conversion and storage applications. However, in order to produce more efficient catalyst supports, modification of graphene oxide is our primary research focus to stick the metal nanoparticles to the graphene surface and also for solution processing of catalyst inks for better electrode fabrication. We successfully modify graphene with various active functional groups for example amine, thiophene, fluorosilane, and RGD peptide. Then, these modified graphene has been used as efficient supports for Platinum (Pt) catalyst nanoparticles. The dispersion of Pt deposited on modified graphene has been enhanced and stable optimized dispersions were obtained in organic solvents. The cyclic voltametry (CV) results of Pt on functional graphene showed a high electrochemical surface area (ECSA) of 147 $m^2/g$ for Pt/GO-RGD compared to Pt/carbon black (Pt/C, 80 $m^2/gPt$) and Pt/GO (99 $m^2/gPt$). Also the functionalized GO/Pt showed higher oxygen reduction reaction (ORR) activity compared to Pt/C. On the other hand, we also fabricated GO/PPy/CB (carbon black) hybrid nanocomposites as catalyst support and deposited Pt nanoparticles. The CV results showed a high ECSA of 153 $m^2/gPt$. Gas diffusion electrode gabrication of the graphene nanomaterials and their use in proton exchange membrane fuel cells (PEMFC) will be reviewed and their electrochemical activity will be discussed further.

P.S.A.14.

# Modeling of optimal parameters of synthesis and sintering of nanostructured NiFeCuW powder

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Electrochemical synthesis of nanostructured NiFeCuW powder is carried out from ammonia solution at current densities: 50 mA/cm$^2$, 100 mA/cm$^2$, 200 mA/cm$^2$, 250 mA/cm$^2$, 300 mA/cm$^2$, 350 mA/cm$^2$, 400 mA/cm$^2$ and 450 mA/cm$^2$. Nanostructured powder of the same chemical composition was prepared by mechanical-chemical milling of mechanical mix of polycrystalline Ni, Fe, Cu and W powders for period of 30 min, 60 min, 90 min, 120 min, 150 min, 180 min, 210 min, 240 min, 270 min, 300 min and 360 min. XRD analysis method was performed in order to characterize all obtained nanostructured powders. It is shown that size of nanocrystallites, defect density and micro-strains in powder is dependent form current density of depositing as well as duration of powder activation.

Thermal-magnetic measurements in the temperature interval from room temperature to 600 ºC, shown that electrochemically obtained powder under current density of 450 mA/cm$^2$ has the best magnetic properties. Powder of the same chemical composition obtained by mechanical activation for 120 min has the best magnetic properties.

It was shown that for all synthesized powders, structural relaxation process is the most intense in the temperature range from 150 °C to 420 °C. The maximum magnetization of all powders, obtained by this method is achieved after annealing at a temperature of about 420 °C for 10 min. It has been found that the magnetization of the powder obtained in the current density depositing of 450 mA/cm$^2$ before annealing is Mo = 5.4 Am$^2$/kg and after annealing at 420 °C is M'=7.1 Am$^2$/kg. Maximum magnetization of powder with activation time of 120 min before annealing is Mo=32.19 Am$^2$/kg and after annealing is M'=36.55 Am$^2$/kg.

Based on the experimental results of thermal-magnetic measurements, we performed mathematical modeling of magnetization depending on the current density of depositing. For powders obtained by mechanical activation we performed mathematical modeling of dependence of the magnetization from the powder activation time.

P.S.A.15.

# The study of the products of off-line pyrolysis of poly(ethylenimine)

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Gas chromatography (GC) and gas chromatography coupled with mass spectrometry (GC/MS) could be useful methods for analysis of nonvolatile samples, like natural and synthetic polymers, if those are subjected to pyrolysis. Polymers are heated at high temperatures that cause fast fragmentation to small volatile products, compounds that could be analyzed by GC and GC/MS. One of the most important points is reproducibility of fragmentation and formation of specific products on the basis of which the structure of pyrolyzed polymers could be identified. Poly(ethylenimine) (PEI) is water-soluble polymer, which is used in many branches of industries, such as industry of detergents, paints, adhesives and glues, paper and cosmetics. It is also used as a flocculant and polyelectrolyte, and it is used in water purification process. However, although the use of PEI is very intense, both in industry and households, its fate in the environment is has been very little studied so far. Also, there is very little information available about the products and mechanism of thermal degradation of PEI.

Identification of the products of pyrolysis of branched PEI was achieved by “off line’’ method at high temperatures, aimed at finding a marker compound, that can be useful for identification of PEI in environmental samples. Samples of PEI (Mn =10,000 g/mol, Mw =25,000 g/mol) are pyrolyzed in a tube oven at three different temperatures (400, 500, 600°C). Constant flow of nitrogen through the system was used to carry pyrolysed products to the recipient flask with dichloromethane. Dissolved mixture was derivatised with acetic anhydride, in the presence of triethylimine and dimethylaminopyridine (DMAP) as catalyst. After derivatization, the products were analyzed by GC/MS. It is found that pyrolizate is complex mixture of compounds, with dominant N,N-diethylamine. Also, in all mixtures is evident presence of different compounds with pyrazine structure.

Off line pyrolysis coupled with derivatization of obtained degradation products and further GC/MS analysis is promising method for determination of PEI in environmental samples. Derivatization of amines, as pyrolytic products, to amides, is crucial step that prevents adsorption of amines at chromatographic column.

P.S.A.16.

# Parameters and sinterability of mullite-$ZrO_2(Y_2O_3)$ nanoparticles prepared by plasma and chemical methods

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Mullite-$ZrO_2(Y_2O_3)$ spherical nanoparticles with diameter in the range of 40-65 nm, containing t-, m-$ZrO_2$ phases and traces of mullite were prepared by using thermal plasma.

Combustion synthesis from appropriate salts water solution was performed in the presence of glycine at 500 ºC during 2 h and additional calcination at 950 ºC. The obtained powder contained mullite and t-$ZrO_2$ phases with crystallite size of 25 and 15 nm respectively.

Molten salts synthesis at 850-900 ºC for 2 h allowed obtain crystalline mullite and t-ZrO2 nanoparticles with crystallite size of 60 nm, 55 nm respectively.

The parameters of prepared nanoparticles and sinterability using spark plasma sintering were compared. The powders produced by plasma chemical synthesis showed higher sinterability. They allowed prepare fine-grained (0.8-1.4 µm) dense materials (99.1%) at 1400 ºC during 3 min.

Acknowledgments: Financial support to this project was provided by National Research Programme (IMIS2).

P.S.A.17.

# Sample preparation method influence on SOP modes in ZnO(Mn)

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The purpose of this work was to study influence of preparation method on optical properties of nanosized powders of ZnO doped with MnO. Nanocrystaline samples were synthesized by calcination and hydrothermal method. These methods allowed obtaining the series of samples with nominal concentration of MnO from 5 to 95% by calcination method and from 5% to 70% of MnO by hydrothermal method. Morphology of all the samples was investigated using scanning electron microscope (SEM), while phase composition and the mean crystalline size were determined by X-ray diffraction. Vibrational properties of investigated samples were studied by Raman spectroscopy.

In samples obtained by calcination method phases of ZnO, $Mn_3O_4$, $ZnMn_2O_4$ and $ZnMnO_3$ with the mean crystalline size (between 9 and 13 nm for $ZnMnO_3$ phases, from 24 to 47 nm for $Mn_3O_4$ phases and above 100 nm for ZnO and $ZnMn_2O_4$ phases) are obtained by XRD analysis. Raman spectroscopy confirmed existence of all phases found by XRD, but also revealed MnO phase whose presence hasn’t been registered with XRD. In the range of 520-575 cm-1 surface optical phonon (SOP) are present.

Composition of hydrothermally obtained samples is quite different. Only presence of ZnO and $ZnMn_2O_4$ phases with the mean crystalline size (between 33 and 99 nm for ZnO and from 16 to 29 nm for $ZnMn_2O_4$ phase) is obtained by XRD analysis. Raman spectroscopy confirmed existence of this two phases found by XRD, but also revealed presence of MnO, $Mn_3O_4$ and $ZnMnO_3$ phases. In the range of 497-538 cm-1 surface optical phonon (SOP) are present. The phonon of registered phase’s exhibit effects connected to phase concentration, while the SOP phonon mode exhibit significant confinement effect. From our result we can see that preparation method have significant influence on dopant incorporation in host lattice and formation of existing phases, but it doesn’t change the basic trend of modes behavior with concentration increase.

P.S.A.18.

# Crystal structure, optical and magnetic properties of ZnO:Fe nanoparticles

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Zinc oxide is one of the most studied materials due to its potential applications in electronics, optoelectronics and spintronics. Actually, spintronics is currently an arising area of research because spin-based multifunctional electronic devices have advantages over the conventional charge-based devices regarding data-processing speed, nonvolatility and higher integration densities. According to a recently published data, ZnO substituted with 3D transition metal (Cr, Mn, Fe, Co, Ni, Cu) are applicable for spintronic due to the room temperature ferromagnetism. Besides, it have been shown that the magnetism of transition metal substituted ZnO is very sensitive to surface defects, particle size, type of the transition metal and concentration of native or artificially introduced defects.

In this study we investigated the influence of Fe concentration in ZnO:Fe nanoparticles on crystal structure, optical and magnetic properties. ZnO:Fe nanoparticles with nominally 5, 10, 15 and 20 at.% of Fe ions were synthesized by microwave processing of a precipitate. The crystal structure and phase purity of the samples were investigated by X-ray diffraction and Raman spectroscopy. Electron paramagnetic resonance (EPR) and Mössbauer studies were carried out to clarify the valence state of the iron ions in the ZnO:Fe crystal structure. The particles morphology and size distributions were characterized by FE–SEM and laser diffraction particle size analyzer, respectively. The optical properties were studied using UV–Vis diffuse reflectance, while the nature of the visible emission in ZnO:Fe were determined by photoluminescence (PL), photoluminescence excitation (PLE) and EPR spectroscopy. The influence of the iron concentration in the ZnO:Fe crystal structure on magnetic properties was studied by a superconducting quantum interference device (SQUID) magnetometer. A series of first principles calculations has been performed to address the influence of the iron concentration on the electronic structure of ZnO:Fe samples.

P.S.B.1.

# Electron structure, valence state Ce(Yb) and magnetic properties of new ternary intermetallic compounds

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In rare earth compounds, where 4f levels are relatively close to the Fermi energy, various anomalous phenomena frequently appear. Most of them can be attributed to hybridization between the 4f states and conduction zones. A mixed-valence (MV) state is one of these phenomena. The MV phenomenon has attracted a great deal of interest during the last several decades in connection with valence fluctuations. In the gas phase most rare earths are divalent, but in the solid state most are trivalent, due to the large cohesive energy gained by promoting a 4f electron into an extended bonding state. The rare earth compounds based on Sm, Eu, Tm and Yb ions frequently exhibit a mixed-valence state consisting of divalent and trivalent valences. In the mixed-valence compounds, therefore, one most also consider the charge degrees of freedom of the 4f ions in addition to the spin and orbital degrees of freedom.

High-energy spectroscopy (XES, XAS and XPS) has been used to study the electron structure and valence states of the new ternary intermetallic compounds with crystallize in the Tb4Rh6Sn18, $ThCr_2Si_2$, $Yb_2Fe_4Si_9$ and $ThMn_{12}$ types. The theoretical calculations have been carried out by means of the ab initio fully-relativistic spin-polarized Dirac linear muffin-tin orbital method. LIII -absorption spectra Ce(Yb) in ternary compounds were obtained at 80K and 300K using a tube spectrometer. The MV state of Ce(Yb) was obtained in the investigation compounds. The measurements were carried out both with classical methods as well with the Mossbauer effect in order to establish parameters of the hyperfine interactions (only for $R_5Fe_6Sn_{18}$(R = Er, Tm, Lu) compounds). A satisfactory agreement between theoretical and experimental data is achieved.

P.S.B.2.

# Influence of different precursor solutions on final characteristics of barium titanate based thin films

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Field of electro ceramics is one of the most popular areas of research in microelectronics. In order to provide lead free materials for different electronic applications, barium titanate has a significant role in this research. Apart from barium titanate, barium strontium titanate is also material with a lot of potential in this field of application. Possibilities for fabrication of a large number of different devices, such as capacitors, MEMS and tunable microwave devices have increased. Due to the trend of miniaturization in microelectronics, thin films are very interesting for investigation. Aim of this work was investigation of influence of solution preparation on final structure of barium titanate and barium strontium titanate thin films obtained with spin coating. Combination of different precursors and solvents was used for preparation of solutions. Barium carbonate and barium acetate were used as barium sources and acetic acid and 2-metoxi ethanol as solvents. Strontium acetate was used as dopant in different concentrations (10, 20, 30 and 40 at.%). Stability of systems was adjusted with DCCA (Drying Control Chemical Additives) and changes in solutions were monitored for different time, from few hours up to few days. Obtained solutions were deposited on previously cleaned silicon substrates by spin coating. After the deposition, films were thermally treated on different temperatures (750, 900, 1000°C). Structures of obtained films were investigated with scanning electron microscopy (SEM), X-ray diffraction (XRD) and Raman spectroscopy.

P.S.B.3.

# YBCO bulk superconductor exposed to air moisture

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The reaction of surfaces of oxygenation cracks of YBCO bulk single- grain superconductor with air moisture was studied. X-ray photo-emission spectroscopy, done on air exposed (001) surfaces, confirmed oxygen bonds related to barium hydroxide. Thermal analyses and mass spectrometry of exposed samples has shown a release of water caused by decomposition of barium hydroxide hydrates during sample heating. The formation of nano-size barium hydroxide phases at the surfaces of oxygenation cracks and morphological changes of these phases at heating were observed with scanning electron microscope.

Acknowledgement: This work was realized within the framework of the projects: New Materials and Technologies for Energetics (ITMS 2 6220220061), Research and Development of Second Generation YBCO Bulk Superconductors (ITMS 26220220041), which are supported by the Operational Programme ‘Research and Development’ financed through the European Regional Development Fund, APVV No. 0330-12, VEGA No. 2/0121/16.

P.S.B.4.

# Computational study of loratadine reactivity in order to understand its degradation properties from the aspect of DFT and MD simulations

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Loratadine (LOR, ethyl 4-(8-chloro-5,6-dihydro-11H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-ylidene)-1-piperidinecarboxylate, $C_{22}H_{23}ClN_2O_2$, 382.88 g/mol, CAS Number 79794-75-5) is an active component of a second generation selective antihistaminic pharmaceutical usually known as Claritin. Frequent usage of this type of pharmaceuticals imposes the need for understanding their fundamental reactive properties. In this study we have theoretically investigated reactive properties of LOR using first of all density functional theory (DFT) calculations that were used to collect the information related to molecule stability, structure, frontier molecular orbitals, quantum molecular descriptors, charge distribution, molecular electrostatic potential surfaces, charge polarization, and local reactivity properties according to average local ionization energy surfaces. According to bond dissociation energies, oxidation is the most likely to happen at piperidine and cycloheptane rings. Also, molecular dynamics (MD) simulations were used in order to understand the interactions with water through radial distribution functions. Collected results provided information important for suggestion of possible degradation compounds.

Acknowledgements: This work has been done thanks to the support received from Schrödinger, Inc. Presented research was done within the framework of projects supported by the Ministry of Education, Science and Technological Development of Republic of Serbia, grant numbers 172042, 171039 and 34019.

P.S.B.5.

# Synthesis and characterization of Pd nanocatalyst at tungsten carbide based support for fuel cells application

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Tungsten carbide was prepared by polycondensation of resorcinol and formaldehyde in the presence cetyltrimethylammonium bromide (CTABr) surfactant. Pd nanocatalyst at this support was synthesized by borohydride reduction method. The obtained materials were characterized by XRD, HRTEM, EELS, XPS and electrochemical measurements. TEM analysis revealed Pd nanoparticles size in the range of a few nanometers, even the clusters of Pd atoms. X-Ray Photoelectron Spectroscopy was applied to determine surface composition of the substrates. The presence of palladium based species was revealed. The catalytic activity for the hydrogen oxidation reaction and oxygen reduction were investigated in 0.5 M $HClO_4$ by cyclic voltammetry and linear sweep voltammetry at the rotating disc electrode. The catalysts' activities were compared to the carbon supported Pd nanoparticles (Vulcan XC 72). WC supported Pd nanoparticles have shown higher CO tolerance, compared even to Pt based catalyst.

Acknowledgements: This work was financially supported by Ministry of Education, Science and Technological Development, Republic of Serbia, contract No. 172054.
The authors would like to acknowledge networking support by the COST Action MP1407.

P.S.B.6.

## Corrosion stability of graphene coatings on metallic substrates

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Cyclic voltammetry (CV), potentiodynamic sweep (PDS) measurements, electrochemical impedance spectroscopy (EIS), scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS) were used to investigate the corrosion stability of graphene coatings on various metallic substrates in 0.1 M chloride solution. The effect of the annealing process before graphene coating deposition on the corrosion stability of the graphene coated substrates was also assessed. Based on the electrochemical measurements and surface analysis graphene coatings grown by CVD can act as a corrosion barrier for metallic substrates, offering corrosion protection by extending the time required for the electrolyte to reach the metallic surface beneath the graphene coating. The results demonstrated that the quality of the deposited graphene layers was affected by the pre-annealing of the metallic substrate. The number of layers and the degree of defects in the synthesized graphene coatings both decreased as the annealing time increased, resulting in larger graphene domains

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P.S.B.7.

## Solid-state reactions in nanomaterials based on monolayered chalcogenides of transition metals

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Monolayered dichalcogenides of transition metals $MX_2$ (X = S, Se, Te; M = Ti, Zr, Mo, W, etc.) have been considered lately as a new and very prospective class of compounds to be used as electronic devices. The compounds are known to exist in two polymorphic modifications H-$MX_2$ and T-$MX_2$. Here we report a theoretical discovery of a transition state TS-$TiS_2$ associated with the reaction H-$TiS_2$→TS-$TiS_2$→T-$TiS_2$ and two transition states associated with two possible reactions T-$MoS_2$→TS-$MoS_2$→H-$MoS_2$.

P.S.B.8.

## SiC and Si-C-N ceramics derived from new siliconorganic polymers

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Polymer-derived silicon carbide (SiC) and silicon carbonitride (Si-C-N) ceramics are of a great interest due to high oxidation stability (up to 1600°C), hardness and a uniform microstructure. Polymer pyrolysis technique is suitable to obtain both bulk ceramics and ceramic matrix for composites reinforced by fibers. It is well known that the chemical composition of Si-C and Si-C-N ceramics and their microstructure depend on many factors such as chemical composition of polymer precursor, heat-treatment parameters, additives etc.

In the present work, the pyrolysis of new type of siliconorganic polymers was studied. Feature of these polymers is the presence of nitrogen atoms along with multiple carbon-carbon bonds that cause the intermolecular cross-linking of the polymer at temperatures about 300°C and increase the ceramic yield. The main steps of polymer pyrolysis were determined, the morphology and phase composition of ceramic products were investigated by modern techniques.

This study was supported by RFBR, research project No. 16-33-60176 mol_a_dk.

P.S.B.9.

## Macroporous conducting cryogels based on polyaniline

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Conducting polymer cryogels were prepared by the oxidation of aniline hydrochloride in frozen reaction mixtures containing a supporting polymer, poly(vinyl alcohol). The resulting composite polyaniline/poly(vinyl alcohol) hydrogels were macroscopically homogeneous, and had macroporous structure with average pore size of the order of 100 µm. The typical conductivity of cryogel swollen with water or acid solution was $10^{-2}$ S $cm^{-1}$. The conductivity has both the electronic and ionic contributions. The molecular structure of polyaniline was confirmed by Raman spectroscopy. The hydrogels can be converted to the corresponding aerogels by freeze-drying. Cryogels are likely to be applied in biomedicine and in supercapacitors.

The financial support of the Czech Science Foundation (16-02787S) is gratefully acknowledged.

P.S.B.10.

## Temperature responsive hydrogels with ethylene glycol propylene glycol pendant chains

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New hydrogels based on different oligo(alkylene glycol) methacrylate (OAGMA) with inverse thermoresponse and volume phase transition temperature (VPTT) were obtained and characterised. Synthesis was performed from monomer-solvent (OAGMA-water/ethanol) mixture using gamma radiation. Characterisation of the hydrogels was performed by swelling, UV-Vis, FTIR, SEM, DSC and in vitro biocompatibility (cytocompatibility and haemolytic activity) investigations. Due to the possibility to combine VPTT close to human body temperature with good biocompatibility, new homopolymeric hydrogel based on EGPG “block” pendant chains showed promising potential for different biomedical applications.

Acknowledgement: This work has been supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (grant No. 172026).

P.S.B.11.

## Nanocomposites of polypyrrole nanotubes and noble-metal nanoparticles

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Polypyrrole nanotubes were prepared by the oxidation of pyrrole with iron(III) chloride in the presence of methyl orange. They were subsequently used as a substrate for the reductive deposition of noble metal particles. Polypyrrole nanotubes with deposited palladium, platinum, rhodium, or ruthenium nanoparticles were characterized by electron microscopy, conductivity, energy dispersive X-ray analysis, and FTIR and Raman spectroscopies. A typical metal content varied between 15–20 wt.%, the particle sizes were of tens nanometers. The catalytic activity of composites was illustrated on the reduction of 4-nitrophenol to 4 aminophenol. The nanotubular morphology of polypyrrole was retained after carbonization at 830 °C. The size of platinum nanoparticles was preserved in samples exposed to 400–500 °C in inert atmosphere. Such temperatures are found to be sufficient for the conversion of polypyrrole to nitrogen-containing carbon.

The financial support of the Ministry of Education of the Czech Republic (LH14199) is gratefully acknowledged.

P.S.B.12.

## Electrical properties of mechanically activated magnesium-titanate ceramics

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In this paper the influence of mechanical activation on electrical properties of magnesium-titanate ceramics has been investigated. Mixtures of MgO and $TiO_2$ powders at a molar ratio $MgO:TiO_2$ = 2:1 were mechanically activated by grinding in a high energy planetary ball mill device. Nonactivated and mixtures treated in planetary ball mill for 5, 10, 20, 40, 80 and 120 minutes were sintered at 1300ºC. The influence of mechanical activation on phase composition and crystal structure has been analyzed by XRD, while the effect of activation on microstructure was investigated by scanning electron microscopy.

Electrical properties were investigated in the frequency range from 1 kHz to 5 MHz by RLC meter. Correlations between capacitance, angle of dielectric losses as well as real and imaginary part of impedance with activation time and polarization mechanism were performed.

P.S.B.13.

## Influence of mechanical activation on the $MgO\text{-}Al_2O_3\text{-}SiO_2$ system with $TeO_2$

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Cordierite $2MgO+2Al_2O_3+5SiO_2$ is frequently used ceramic material, that is commonly used as a carrier of electrical components due to its low dielectric constant (~ 5), and low temperature thermal expansion coefficient ($20\bullet10^{-7}$ $^{o}C^{-1}$). In order to accelerate the process of sintering, 5.00 mass% $TeO_2$ was added to the starting mixtures. System was tested in two parallel mixtures, one with no added additives, and the other one with $TeO_2$. The mechanical activation of the both mixtures was performed in a high-energy ball mill in time intervals from 0 to 40 min with ball to powder mass ratio 1:40. The particle size analysis (PSA) was employed in order to determine the changes in the particle size of the mechanically treated powders. The phase composition of the starting powders as well as microstructures was analyzed by the means of X-ray diffraction method and SEM.

P.S.B.14.

## Temperature dependence of thermal conductivity of two-layered graphene

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The heat transport of the two-layer graphene is analyzed, by using different mechanisms of the intra-layer phonon scattering (of both in-plane and out-plane phonons of the graphene mono-layers on defects, borders, phonons, and electrons of the corresponding graphene mono-layers) and inter-layer phonon scattering (of out-plane phonons of the one graphene mono-layer on out-plane phonons of another graphene mono-layer). To investigate thermal conductivity of the two-layer graphene, the Boltzmann transport equation in the approximation of relaxation time is hereby used. Temperature dependence of thermal conductivity of the two-layer graphene is presented graphically in the range of 0 – 400 K, and compared with the available literature data.

P.S.B.15.

## The electrical resistance decay of a metallic granular packing

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We report on measurements of the electrical conductivity on a two-dimensional packing of metallic disks when a stable current of 1 mA flows through the system. At low applied currents, the conductance $\sigma$ is found to increase by a pattern $\sigma(t) = \sigma\infty - \Delta\sigma E\alpha[-(t/\tau)\alpha]$, where $E\alpha$ denotes the Mittag-Leffler function of order $\alpha \in (0, 1)$. By changing the inclination angle $\theta$ of the granular bed from horizontal, we have studied the impact of the effective gravitational acceleration $geff = g \sin \theta$ on the relaxation features of the conductance $\sigma(t)$. The characteristic timescale $\tau$ is found to grow when effective gravity geff decreases. By changing both the distance between the electrodes and the number of grains in the packing, we have shown that the long term resistance decay observed in the experiment is related to local micro-contacts rearrangements at each disk. By focusing on the electro-mechanical processes that allow both creation and breakdown of micro- contacts between two disks, we present an approach to granular conduction based on subordination of stochastic processes. In order to imitate, in a very simplified way, the conduction dynamics of granular material at low currents, we impose that the micro-contacts at the interface switch stochastically between two possible states, “on” and “off”, characterizing the conductivity of the micro-contact. We assume that the time intervals between the consecutive changes of state are governed by a certain waiting-time distribution. It is demonstrated how the microscopic random dynamics regarding the micro-contacts leads to the macroscopic observation of slow conductance growth, described by an exact fractional kinetic equations.

P.S.B.16.

# Analyses of commercially and laboratory produced ODS steels

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The presented paper is focused on the investigation of the microstructural changes caused by manufacturing process and ion implantation in commercially and laboratory produced ODS steels. Via differences in Positron annihilation spectroscopy parameters, the changes due to differences in chemical composition and preparing technology of studied advanced alloys can be clearly evaluated. The results of Mössbauer spectroscopy contribute to the complex information about studied materials via unique characteristics as micro-magnetic properties or homogeneity of admixtures distribution in steels. Furthermore the radiation resistance of these materials was studied via helium ions implantations by Magnetic Barkhausen Noise and Atomic Force Microscopy measurements. The combination of the proposed techniques will assure the complex information about different microstructural changes of studied materials (size of vacancy type defects, magnetic properties, lattice phases, ect.) in the form of quantitative and qualitative characteristics.

The laboratory produced ODS steels were received from laboratories involved in the Coordinated Research Project F11014 "Benchmarking of Structural Materials Pre-selected for Advanced Nuclear Reactors". Namely from India (IGCAR), Russia (Bochvar Institute), Korea (KAERI) and Japan (Kyoto University). The commercially produced steels used in this work were PM2000 and MA 956.

P.S.B.17.

## Ni-based alloys coatings for high temperature applications

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Directions of the development in the power industry, is related to the construction and the building of the power plants with a higher efficiency than the previous one and simultaneous reduction of the emission pollutions to the environment and air.
This study is focused on the high-temperature corrosion resistance of boiler Inconel nickel alloys like Inconel 625 and Inconel 686. Results indicated that corrosion wear of Ni-base coating depend on the chemical composition of combustion products. The combustion of waste produced the ashes and aggressive gasses containing: sulfur, chlorine and oxygen.
This work presents the causes and mechanisms of high-temperature corrosion of boiler elements during the waste incineration. Results of Ni-coated boiler tubes exposed the ashes and high temperature were performed using scanning and transmission electron microscopy supported by energy dispersive X-ray spectroscopy and HRTEM. On the surface of the Ni-base coating were observed $Cr_2O_3$. Paper presents the nature of grow and the changes of chemical composition of $Cr_2O_3$.

P.S.B.18.

## Effects of retrogression and reaging treatments on the mechanical characteristics of alloy EN AW 7049A-T6

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The retrogression and reaging (RRA) treatment is heat treatment process applied on the high strength 7xxx serie aluminum alloy in T6 temper condition, to provide significant improvement of the stress corrosion resistance without or with small loss in its strength. The paper presents the influence of RRA treatment on the mechanical properties (hardness and tensile properties) of the aluminum alloy EN AW-7049 in the T6 condition. The retrogression heat treatment was performed at various temperatures and times, while reaging of retrogressed alloy was performed at 120 °C for 24 hours. It has been found that increase the temperature and time of retrogression hardness and strength of the alloy decrease compared to the initial T6 condition.

P.S.B.19.

# Characteristics of stress distribution in the case of single LAP joint of two composite plates

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Stress distribution in the case of single lap joint of two composite plates is analyzed using the finite element method. Analyzing obtained results, it can be concluded:

- stresses sx , sy and txy are practically constant with respect to z coordinate,
- stresses sz , tyz and txz change with z coordinate, but their intensity's are much smaller than first three.

The situation is very similar to model of so called "plane strain state" defined in the Theory of Elasticity.

In this case composite material must be defined as orthotropic.

P.S.B.20.

# OLE of tribology effects on cup anemometer classification

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The advanced methods of wind energy potential assessment for planning wind electricity plants are mostly based on new laser technology. The so called cube system allows for 3D wind speed measurements, but the cup anemometer, invented 170 years ago, is still the reference instrument in wind energy conversion field. A cup anemometer acts as a converter of wind kinetic energy to rotor rotation energy like a vertical axis wind turbine. To prepare a bankable document for a wind farm investment, the use of high quality cup anemometers is required according the accepted classification. Classification system for quantification of systematic errors of cup anemometers was developed and used to derive an uncertainty estimate from a classification index number. The output signal of a cup anemometer depends on the relative contribution of horizontal and vertical wind speed components at the terrain so class A condition corresponds to flat terrain sites, while class B corresponds to complex terrain sites. The selected cup anemometer is classified inside both groups by the class index k that bounds the maximum anemometer error. In this paper, the Angular Speed Decrement model (ASD), which allows for monitoring the anemometer friction characteristics during long-term measurements was applied for calculation of the relative contribution of friction and aerodynamic effects to the offset of two types of NRG anemometers: NRG #40 and NRG class 1. Both anemometers have the same rotor geometry, which means nearly the same aerodynamic characteristics, but different tribological characteristics of the shaft-bearing pair. The shaft of NRG #40 anemometer is made of fully hardened beryllium copper and bearing of self-lubricating modified Teflon, while in case of NRG class 1 anemometer the ball bearing was used. The difference in frictional torque due to different tribological characteristics of shaft-bearing systems results in a small but improved classification index in case of ball bearing system. During long term operation, the friction characteristics of NRG #40 anemometer were changed and some kind of continuous degradation of performance was observed. Several periodic recalibration of NRG #40 anemometer revealed the change of the slope and the offset of calibration curve and simulation of output signal deviation resulted in small change of classification index. Data from long term operation of NRG class 1 anemometer were not available, but in principle, a small change of classification index during long term anemometer operation may be expected.

P.S.B.21.

# Monte Carlo simulations of He+ in CF4

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Cold plasmas are often exploited in new technologies where they favorably offer non-intrusive production or modification of various substances. In this paper we present a new method to simply obtain the elastic momentum transfer cross section which predicts a maximum of reduced mobility and its sensitivity to temperature variation at low energies. We first determined the transport cross section which resembles mobility data for similar closed shell systems by using the Monte Carlo method. Second, we selected the most probable reactive processes and compiled cross sections from experimental and theoretical data. At the end, elastic momentum transfer cross section is obtained by subtracting the compiled cross sections from momentum transfer cross section, taking into account effects of the angular scattering distributions. Finally, in such a way the cross section set determined is used as an input in a final Monte Carlo code run, to calculate the flux and bulk reduced mobility for He+ + $CF_4$ which were discussed as a functions of reduced electric field E/N ( N-gas density) for temperature T=300 K.

P.S.C.1.

# Characterization of graphite-encapsulated iron nanoparticles synthesized by milling-assisted low-pressure chemical vapor deposition

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Graphite-encapsulated Fe nanoparticles are synthesized using a combined method of high-energy ball milling and low-pressure chemical vapor deposition (LPCVD). We use a planetary ball mill to grind $Fe_2O_3$ and graphite powders to reduce their particle sizes, increase their surface areas and distribute them more homogeneously. Then, LPCVD is performed at a pressure of ~0.57 Torr in a tube furnace under a $CH_4/H_2$ atmosphere at 1050 °C for 1 and 3 h. As-synthesized particles are purified in a 2 M HF acid solution to obtain graphite-encapsulated Fe nanoparticles. Characterization investigations are performed using X-ray diffractometry (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM) and alternating gradient magnetometry (AGM). XRD reveals the presence of BCC Fe and FCC (Fe, C) phases without residual iron oxides. SEM proves the homogeneous distribution of the milled $Fe_2O_3$ and graphite powders, and their powder form, after LPCVD in comparison with the bulk form of non-milled powders. High resolution TEM shows all nanoparticles have at least eight graphitic layers around an Fe core with a size range of 20-300 nm. Magnetic measurements indicate that the nanoparticles exhibit soft ferromagnetic behavior with low saturation magnetization and coercivity values of 17 emu/g and 106 Oe, respectively. The chemical stability of the particles is tested by suspending the graphite-encapsulated Fe nanoparticles in a corrosive 2 M HCl acid solution for 12 h under sonication. The graphitic shells do not degrade, nor is there evidence of core dissolution or shell discontinuity. Thus these nanoparticles show interesting properties and are stable in an acidic environment.

This research is funded by the Center for Cancer Nanotechnology Excellence for Translational Diagnostics, an NCI-NIH U54 grant (# 1U54CA199075).

P.S.C.2.

# Structures and properties of quasi-onedimensional vanadium and niobium sulfides with Peierls distortion

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Crystal and electronic structures and transport properties of several quasi-onedimensional semiconducting compounds – known $VS_4$, $NbCl_4$, $NbS_3$ and hypothetical $NbS_4$, $VS_3$ are studied by means of modern physical methods (X-ray single crystal, density functional method, electronic conductivity). Characteristic feature of these compounds containing metal ions with d1 electronic configuration is formation of binuclear M-M clusters in metal chains with localization of two electrons on metal-metal bonds (two electrons two centres 2e2c bonds). Comparative analysis of chemical bonding and charge distribution among all these compounds reveals the possible origins of structural instability of $NbS_4$ and $VS_3$.

The work was supported by Russian Science Foundation (Grant 14-13-00674).

P.S.C.3.

# Aqueous sol-gel route toward selected quaternary metal oxides with single and double perovskite-type structure containing tellurium

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Highly crystalline $SrFe_{2/3}Te_{1/3}O_3$, $Ba_3Fe_2TeO_9$ and $Ba_2NiTeO_6$ have been synthesized by using a specially developed sol-gel route methodology, reducing the time needed using solid-state routes and resulting in high reaction yield up to 75 %. These materials have been studied by X-ray powder diffraction (XRPD), scanning and transmission electron microscopy, Raman spectroscopy, dielectric and magnetic measurements. At room temperature, the crystal structure of $SrFe_{2/3}Te_{1/3}O_3$ is cubic, space group Pm-3m, with a = 3.9373(2) Å, whereas $Ba_3Fe_2TeO_9$ crystallizes in the hexagonal crystal system, space group P63/mmc, a = 5.7691(4) Å and c = 14.208(1) Å. The third studied perovskite $Ba_2NiTeO_6$ crystallizes in trigonal R-3m space group with a = 5.7974(4) Å and c = 28.599(2) Å. Based on structural characterization results, the obtained single and double perovskite crystallites are nearly in nanometer regime, ranging from 45 to 164 nm, building micrometer sized particles with visible well-faceted hexagonal morphology. Magnetic measurements show the onset of ferromagnetic ordering at relatively high temperature of 667 K for the $SrFe_{2/3}Te_{1/3}O_3$, whereas $Ba_3Fe_2TeO_9$ and $Ba_2NiTeO_6$ show anti-ferromagnetic ordering below 80 and 8.6 K, respectively. The measured room temperature dielectric constants are in the range between 15 and 77.

P.S.C.4.

### Thiol click chemistry on gold-decorated $MoS_2$: elastomer composites and structural phase transitions

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We have shown a procedure for decorating $MoS_2$ flakes from chemical exfoliation with AuNPs. TEM images confirm the crystal structure of gold and show that the AuNPs, with typical diameters around 2 nm only slightly coalesce upon thermal treatment at up to 400 °C. Subsequently, we have found that PMMS enables the dispersion of both metallic and semiconducting flakes in the same solvent, and used optical absorption and Raman spectroscopy to show transformation from the metallic to the semiconducting phase without restacking both in dispersion and as fillers of an elastomer nanocomposite. Finally, by using different flakes (decorated and undecorated, different defect content) and PMMS with different degrees of thiolation, we identified the interaction between the thiol groups and the AuNPs as the driving force for the nanocomposite formation. The excellent optical quality of the transparent elastomeric composites of $MoS_2$ in PMMS shows promise for non-linear optical applications, such as saturable absorbers or optical limiters.

P.S.C.5.

### Positronics of sub-nanometer-structured functional materials

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The methodological possibilities of positron annihilation lifetime spectroscopy (PALS) applied to characterize different nanomaterials are analyzed. The first part of report deals with time-dimension relations followed from application of positron-electron interaction formalism to structurally homogeneous media, such as those composing host matrices for embedded nanoparticles. The second part concerns fundamentals of PALS applied to inhomogeneous nanoparticle-embedded substances. The algorithm to treat PALS data for such substances within three-state trapping model evolving competitive channels of positron and positroniun (bound electron-positron atom) annihilation is presented. The developed approach to the problem of void filling in the “host-guest” chemistry is justified at the examples of organic-inorganic nanocomposites, crystallization/ceramization-affected nanoinclusions in phase-separated glassy matrices and intrinsic nanoinhomogeneities in network glass formers.

P.S.C.6.

## Colloidal dispersions of zirconium and titanium trisulfides

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Transition metal trichalcogenides $MQ_3$ (M=Ti, Zr, Hf, Nb, Ta; Q=S, Se, Te) are known due to their electrophysical properties (semiconducting or metallic behavior, some of them demonstrate Peierls transition). These features arise from quasi-one-dimension crystal structure of $MQ_3$. Additionally crystal structures of these compounds are layered, the $MQ_3$ layers are stacked together via Q…Q van der Waals contacts. Thereby $MQ_3$ may be dispersed to nanosized form. In this work we have prepared $ZrS_3$ and $TiS_3$ colloidal dispersions via ultrasonication in organic media and $MQ_3$ films from these dispersions, which are suitable for conductivity measurements. Here we discuss obtaining the $ZrS_3$ and $TiS_3$ sols and film preparation, their description and characteristics.

Acknowledgements: The work is supported by Russian Foundation for Basic Research (Project 16-33-00577 mol_a)

P.S.C.7.

## Investigation of rheological properties of barium titanate inks and adaptation to requirements of inkjet printing

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Inkjet printing is popular method for production of very different types of thin films in electronic industry. In contrast to lithography, inkjet printing is much cheaper and simpler method for fabrication of complex forms. Even though lithography is still more precise than printing, this method have significant place in production of different electronic devices in thin film form. All inkjet printing devices have some requirements such as specific values of viscosity, surface tension and particle size of the ink. Aim of this work was adaptation of rheological properties of barium titanate inks to requirements for inkjet printing with Dimatix printer (DMP-3000). Basically, barium titanate inks were prepared from barium carbonate, tetrabutyl orthotitanate and acetic acid which were used as solvent. Stability of inks was adjusted with concentration of barium and titanium ions, addition of DCCA (Drying Control Chemical Additives) such as glycerin and formamide, and addition of another solvent in system (2-methoxyethanol). Influence of concentration, additives and solvents on inks stability, viscosity and surface tension was investigated. After rheological characterization, inks with required values of viscosity and surface tension were selected and printed on previously cleaned silicon substrates. All printed films were sintered on 750°C. Structural characteristics of films were investigated with optical microscopy, scanning electron microscopy (SEM), X-ray diffraction (XRD) and Raman spectroscopy.

P.S.C.8.

## Sputter-deposited Fe/Al thin superlattices: scanning of non-magnetic layer thickness

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Fe/Al thin multilayer films were produced by sputtering technique. The effect of different thicknesses of non-magnetic (Al) layers on the magnetic properties of the thin multilayer films was investigated. The thickness of Fe layers was 5 nm and total film thickness was 200 nm whereas the thickness of Al layers was adjusted as 95 nm, 35 nm and 7.5 nm considering different bilayer numbers. Atomic Al contents of the multilayers were 71 %, 40 % and 20 % for Al layer of 95 nm, 35 nm and 7.5 nm, respectively. The rest of the films were Fe atoms. A mixture of body centered cubic (bcc) of Fe and face centered cubic of Al structure turned to a bcc structure of Fe when the thickness of Al layers and hence the Al content decreased. Saturation magnetization increased with decreasing Al content and coercivity values altered irregularly.

P.S.C.9.

## Effect of IF-$WS_2$ nanoparticles addition on physical-mechanical and rheological properties and on chemical resistance of water-based paints

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Transition-metal dichalogenides ($MoS_2$, $WS_2$, $NbS_2$, etc.), due to their excellent mechanical properties, are used for a wide range of applications, including aerospace and automotive technology, load bearing and release mechanisms, as solid lubricants, corrosion protection etc. In the form of inorganic fullerene-like particles, with unique morphology, spherical and closed structure, they possess a chemical inertness and a high elasticity. Due to these exceptional characteristics, inorganic fullerene-like particles, such as tungsten disulfide IF-$WS_2$, are recognized as promising materials and promising fillers of the composites and are extensively studied for their ability to control wetting, adhesion, lubrication on surfaces and interfaces, and to achieve good corrosion resistance. In this paper, a possibility is examined to improve properties of water-based paints by adding nanoparticles of IF-$WS_2$. Since they have low % VOC (volatile organic compound), water-based paints are eco-friendly substitute for common polymeric coatings, and nowadays it is very important to introduce their usage as much as possible. IF-WS2 were dispersed in paint by ultrasonic irradiation. Physical-mechanical properties and chemical resistance were examined. The following properties were compared for paint without and with IF-$WS_2$ nanoparticles: hardness, flexibility, elasticity, adhesion, abrasion resistance, IR reflection. Also, resistance to salt atmosphere and salt water were compared. The effect of adding IF-$WS_2$ on rheological properties of the paints has been examined using Dynamic Mechanical Analysis (DMA), observing viscosity as the function of the shear rate.

Acknowledgement: The authors thank to the Ministry of Education, Science and Technological Development of Republic of Serbia for the financial support of the research through the project TR 34034 and to the Military Technical Institute for the material and technical support

P.S.C.10.

## Nanocrystalline boehmite obtained at low temperature

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In this work boehmite powders were synthesized starting from sodium aluminate solution prepared from Bayer liquor. The neutralisation of sodium aluminate solution was performed with the use of sulphuric acid, while glucose was added in the starting solution. In this way, the single phase nanocrystalline boehmite was obtained. Powder X–ray diffraction (XRD), Fourier–transformed infrared spectroscopy (FT–IR), scanning electron microscopy (SEM) and low–temperature nitrogen absorption studies were employed to trace the formation boehmite powders. Addition of glucose has a pronounced effect on development of uniform structure of powder with narrow particle size distribution and high surface area. As–synthesized boehmite powders have high surface area (around 300 $m^2/g$) and the average crystallite size less than 5 nm. The results showed that the properties of the powders (structure, morphology) are influenced by the initial concentration of sodium aluminate solution, as well as by the concentration of glucose.

P.S.C.11.

## Chromatic discretization and selectivity in optical properties of whole crystalline nanofilm-structures in IR region

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Based on microscopic (exciton) theory of optical properties of ultrathin molecular crystalline films, the absorption, reflection and transparency indices were formulated and presented in the function of frequencies of external electromagnetic field in near IR region. We have determined and analyzed optical properties relations for the whole film structure based on the consideration for multiple reflection, absorption and transparency in those multilayered structure. The three-layered dielectric nanofilms with different boundary conditions on surfaces were analyzed and some discrete resonant absorption lines were obtained. Their number, position and distribution depend on the boundary parameter values, and give a great contribution in optical engineering of nanostructures, especially in technology of designing of new electronic and photonic equipment, and for nanoparticles construction for drug carrier/delivery in nanomedicine.

This paper was partly financed by the Ministries of the Serbia (ON-171039; TR-34019), Republic of Srpska (19/6-020/961-16/15) and Vojvodina (114-451-2092/2016-03).

P.S.C.12.

# Effect of IF-$WS_2$ nanoparticles addition on thermo-rheological and mechanical behavior of aramid/phenolic resin/PVB composite material

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Different thermoplastic polymers or thermosetting resins are used as impregnation of aramid fabrics in production of personal ballistic protection products, and a combination of phenolic resin with PVB is often used. Transition-metal dichalogenides, due to their excellent mechanical properties, are used for a wide range of applications, including aerospace and automotive technology, load bearing and release mechanisms, etc. Their fullerene-like nanoparticles, having spherical closed structure, possess a chemical inertness and a high elasticity. Due to these characteristics, inorganic fullerene-like particles, such as tungsten disulfide, IF-$WS_2$, are recognized as promising fillers of the composite materials. In this paper a possibility is examined of using IF-$WS_2$ nanoparticles in aramid/phenolic resin/PVB composite material for improving its thermo-rheological and mechanical properties. Composite samples were made using aramid fabric coated with phenolic resin, poly (vinyl butyral), PVB, and nanoparticles of IF-$WS_2$. The quality of aramid fabrics impregnation with PVB/phenolic resin/$WS_2$, as well as the nanoparticles dispersion and deagglomeration in matrix of PVB/phenolic resin was analyzed by scanning electron microscope (SEM). The effect of adding $WS_2$ on thermo-rheological and elastic properties of the composites has been examined using Dynamic Mechanical Thermal Analysis (DMTA) in a defined temperature range. The storage modulus and loss modulus as a function of temperature for the studied composites were observed, as well as the mechanical loss factor. Fracture toughness is also tested by instrumented Charpy impact test.

Acknowledgement: The authors thank to the Ministry of Education, Science and Technological Development of Republic of Serbia for the financial support of the research through the projects TR 34011 and TR 34034.

P.S.C.13.

# Microstructure characterization of friction stir welded joints made from ultrafine grained aluminium

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Severe plastic deformation processes are modern techniques to produce materials with grain size reduced well below 1 μm. It causes an increase in mechanical properties, which is desirable especially in lightweight metals such as aluminium. Enhancement in mechanical properties is caused by elevated amount of grain boundaries, which behave as obstacles for moving dislocations. However, such materials feature limited thermal stability. Therefore, advanced joining techniques are required to preserve refined microstructure. In the present study, Incremental Equal Channel Angular Pressing and Friction Stir Welding have been chosen as deformation and joining techniques, respectively. Obtained joints were of good quality and they were investigated in order to reveal microstructural changes in the base materials during joining. For this purpose EBSD in SEM and TEM were used. The observations revealed ultrafine grains with high density of dislocations for base materials while the joints exhibit few micron equiaxial grains.

P.S.C.14.

# Synthesis of colloidal NIR-luminescent nanoparticles of rare-earth fluorides using microwave-hydrothermal treatment

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One of the main advantages of hydrothermal treatment is the possibility to synthesize highly crystalline and hydrophilic nanoparticles with predetermined size and narrow size distribution in the form of stable water colloids. This is specifically important in the case of synthesis of nanoparticles for various biomedical applications from biolabelling, bioimaging, and biodetection, to drug delivery and hyperthermia for cancer treatment. In this presentation we try to summarize our efforts in the field of microwave-hydrothermal synthesis of colloidal solutions of Nd-doped NIR-luminescent nanoparticles of various rare-earth fluorides. We show that due to volumetric and uniform heating microwave irradiation allows to obtain easily dispersible and highly crystalline nanoparticles with controlled size and morphology. We discuss specific features of hydrothermal treatment under microwave irradiation and possibilities to improve functional properties of the synthesized nanoparticles.

This work was supported by RSF (grant #16-12-10077).

P.S.E.1.

## Synthesis, characterization and biological application of opto-magnetic nanocomposites with up-converting properties based on $NaYF_4$&$Fe_3O_4$@$SiO_2$ nanoparticles

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The main aim of our research was the synthesis and optimization of the $NaYF_4$&$Fe_3O_4$@$SiO_2$ nanoparticles and testing biological application of the material.

We obtained nanoparticles with optical properties based on the yttrium sodium fluoride doped with the rare earth ions (e.g. ytterbium, erbium, thulium). Hexagonal $\beta$-$NaYF_4$: $Yb^{3+}$, $Ln^{3+}$ nanoparticles up-convert near infrared to visible light. Range of the emission light could be tuned according to composition of the doping metal ions. When we doped the $NaYF_4$ by Tm-Yb pair we obtained the blue and red light after the 980 nm excitation. When we doped the $NaYF_4$ by Er-Yb pair, we obtained the green and the red light as a result of the NIR excitation. Biomarkers based on the NIR excitation allow to imaging deep tissue due to a low NIR absorption by the biological molecules and lack of the autofluorescence. We observed the nanoparticles inside the living cells without any apparent luminescence of the biological components of the cells after the NIR excitation and the visible detection. The nanoparticles are non-toxic for the HeLa cells which we study by MTT Assay.

Magnetic properties of the superparamagnetic iron oxide nanoparticles (SPIONs) can be applied in hyperthermia therapy. The nanoparticles cause increase of temperature under alternating magnetic field which lead to the cancer cells damages. These nanoparticles can be used as contrast agents in Magnetic Resonance Imaging. We synthesized and optimized the $Fe_3O_4$ nanoparticles with the 6 nm size. These nanoparticles have superparamagnetic properties in room temperature. These nanoparticles we applied in the hyperthermia measurements and observed the increasing of temperature to 40 °C after 30 min in 50 mg/ml in octadecane.

The coating of both materials inside single $SiO_2$ shell opens the way to create multifunctional nanocapsules applicable in photodynamic and hyperthermia therapies.

Acknowledgements: The research was partially supported by the project „Development of the cluster center of biomedical engineering" implemented under Economy Operational Program (project no. UDA-POIG.05.01.00-00), the EU Research Project FP7-People-2012-IRSES-BRASINOEU (Grant Agreement Number: PIRSES-GA-2012-318916), the grants of PNSC 2013/11/B/NZ1/00089, NN UMO-2013/08/A/ST3/00297, DEC-2012/07/B/ST5/02080 and DEC-2014/15/D/ST5/02604. This work has been done in the NanoFun laboratories co-financed by the European Regional Development Fund within the Innovation Economy Operational Program, the Project No. POIG.02.02.00-00-025/09/. This research was also co-financed by the Swiss National Science Foundation through the Nano-Tera.ch Focused Project (NTF), 'NanoUp'.

P.S.E.2.

## Development and characterization of Mg-containing hydroxyapatite, β-tricalcium phosphate and biphasic calcium phosphate bioceramics

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Calcium phosphates (CaPs), e.g. hydroxyapatite, β-tricalcium phosphate due to their unique properties – bioactivity and/or biodegradability, osteoconductivity, are considered to be promising bone grafts. CaPs present themselves as prime materials for modification, aiming for improvements on physicochemical and biological aspects of novel graft. Nowadays interest is turning towards modified synthetic CaPs involving the addition of various elements. The goal of our work is to develop Mg-containing CaP bioceramics and to evaluate an effect of the Mg addition on physicochemical characterization in particle and bulk level, as well as asses a biological performance of the Mg-containing CaP bioceramics.

Results confirmed that CaP bioceramics with various and reproducible phase and chemical composition were obtained through the precipitation of precursors followed by uniaxial compaction and sintering (1100 ºC, 1 h). The Mg-containing CaP bioceramics show advisable bioactivity with osteogenic progenitor cells and have good cytocompatibility, showing no negative effects on cells growth and proliferation.

Acknowledgment: This work has been supported by the National Research Programme No. 2014.10-4/VPP-3/21 "MultIfunctional Materials and composItes, photonicS and nanotechnology (IMIS2)" Project No. 4 "Nanomaterials and nanotechnologies for medical applications".

P.S.E.3.

## Design and characterization of hydroxyapatite/poly(vinyl alcohol) nanocomposite coated titania scaffolds for bone repair

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Main requirements of porous scaffolds used for bone tissue engineering are easy cell penetration, distribution and proliferation, permeability of culture medium, in vivo vascularisation, adequate mechanical properties, controlled biodegradation, and ease of fabrication. Thus the work is focused on the preparation of novel tissue engineering scaffolds with suitable mechanical properties and favorable microstructure based on biodegradable polymer/inorganic nanocomposite and porous ceramic. Macroporous titania scaffolds with pore size ranging from 100 to 500 μm were obtained by polymer replica method. Uniform, a few μm thin coating composed of hydroxyapatite synthesized in presence of poly(vinyl alcohol) were obtained on the porous titania scaffolds through vacuum-assisted impregnation method while the original macroporosity and open pore structure of the titania scaffolds were maintained. The mechanical strength, degradation and in vitro bioactivity of the scaffolds were characterized.

Acknowledgment: This work has been supported by National Research Programme No.2014.10-4/VPP-3/21(IMIS2) Project No.4.

P.S.E.4.

## Color of dental composite restorations related to dentin substituents

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Composite layer thickness may affect the esthetic appearance of the final restoration. The aim of this work was to investigate the effect of novel dentin substituents on the color of final composite restorations. Standardized specimens of dentin substituents: HAp inserts (proprietary material), Biodentin (Septodont) and EverX Posterior (GC) were covered with composites Filtek $Z_{25}0$, $Z_{55}0$ (3M ESPE) or Gradia Direct (GC) of different shade (A1/A3) and layer thickness (0.6-2 mm) which were then light-cured. Color was measured using a spectrophotometer (Vita EasyShade Advance 4.0, VITA). Color of HAP and Biodentin significantly differed from composites ($p<0.05$). HAP had a greater effect on composite color of 0.6 mm layer than Biodentin and EverX Posterior ($p<0.05$). Dentin substituents affected the final restoration color irrespective of composite type, shade and thickness. In general, 2 mm is the recommended thickness of the top composite layer mimicking the effect of dentin substituents.

P.S.E.5.

# Synthesis, characterization and antimicrobial activity of pentagonal bipyramidal Fe(III) complexes with 2,6-diacetyl- pyridine bis(trimethylammoniumacetohydrazone)

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In the template condensation reaction of 2,6-diacetylpyridine and Girard¢s T reagent in the presence of Fe(III) and ammonium thiocyanate the $[Fe_2(L)_2(NCS)_4][Fe(NCS)_5(H_2O)]\times4H2O$ and $[Fe(L)(NCS)_2]SCN\times2H_2O$ complexes were obtained and characterized by X-ray single-crystal analysis, IR spectroscopy and elemental analysis. The structural unit of complex $[Fe_2(L)_2(NCS)_4][Fe(NCS)_5(H_2O)]\times4H_2O$ consists of two complex cations $[Fe(L)(NCS)_2]+$ of PBPY-7 geometry, complex anion [Fe(NCS)5(H2O)]2- of octahedral geometry and four non-coordinated water molecules. The structural unit of complex $[Fe(L)(NCS)_2]SCN\times2H_2O$ consists of complex cation $[Fe(L)(NCS)_2]+$ of PBPY-7 geometry thiocyanate counter anion and two non-coordinated water molecules.

Antimicrobial activity of ligand, Fe(III) complexes and corresponding salt was tested against seven standard strains of bacteria Staphylococcus aureus (ATCC 6538), Staphylococcus epidermidis (ATCC 1228), Bacillus subtilis (ATCC 6633), Escherichia coli (ATCC 10536), Klebsiella pneumoniae (ATCC 13883), Pseudomonas aeruginosa (ATCC 9027), Salmonella abony (ATCC 6017) and one strain of yeast Candida albicans (ATCC 10231). Results of antimicrobial activity showed that activity of complex $[Fe_2(L)_2(NCS)_4][Fe(NCS)_5(H_2O)]\times4H_2O$ was higher than the activity of complex $[Fe(L)(NCS)_2]SCN\times2H_2O$. Complex $[Fe_2(L)_2(NCS)_4][Fe(NCS)_5(H_2O)]\times4H_2O$ exhibited moderate activity against all tested antibacterial strains, while the activity against yeast was low.

P.S.E.6.

# Synthesis and development of polymeric scaffolds based on (meth)acrylates for tissue regeneration applications

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The discovery of new biomaterials and scaffold fabrication techniques enhance the development of tissue engineering. The structural properties of scaffolds affect cell response and have to be designed to support cell adhesion, proliferation and differentiation. In this study, the investigated scaffolds were synthesized using combined technique which includes microwave and photo-irradiation. Natural polymers gelatin and alginate because of their great resemblance to extracellular matrix elements, as well as 2-hydroxyethyl (meth)acrylate due to their mechanical properties were used. The chemical structure of investigated matrices was studied by Fourier transform infrared spectroscopy, while their morphology was examined by scanning electron microscopy. Various architectural parameters of the scaffolds important for tissue engineering (porosity, pore size, interconnectivity) and swelling behavior were discussed. These novel matrices have potential tissue regeneration applications as scaffolds due to their unique architecture and physico-chemical properties.

Acknowledgment: This work has been supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Grant No 172062) and the SCOPES programme of the Swiss National Science Foundation (SNSF) and the Swiss Agency for Development and Cooperation (SDC) (Grants No IZ73ZO_152327/1). Bojan Božić would like to thank the program “Start Up for Science”, supported by Phillip Morris.

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66.017/.018(048)

MATERIALS Research Society (Beograd). Conference (18 ; 2016 ; Herceg Novi)
Programme ; and The Book of Abstracts / Eighteenth Annual Conference
YUCOMAT 2016, Herceg Novi, September 5-10, 2016 ; organised by Materials
Research Society of Serbia, Belgrade ; [editors Dragan P. Uskoković and
Velimir Radmilović]. - Belgrade : Materials Research Society of Serbia,
2016 (Herceg Novi : Biro Konto). - XXXVI, 109 str. ; 23 cm

"This conference is held in honour of Prof. Dejan Raković's 65th birthday"
--> impresum. - Tiraž 220.

ISBN 978-86-919111-1-9
1. Materials Research Society of Serbia (Beograd)
a) Наука о материјалима - Апстракти b) Технички материјали - Апстракти
COBISS.SR-ID 225349644

MATERIALS RESEARCH SOCIETY OF SERBIA
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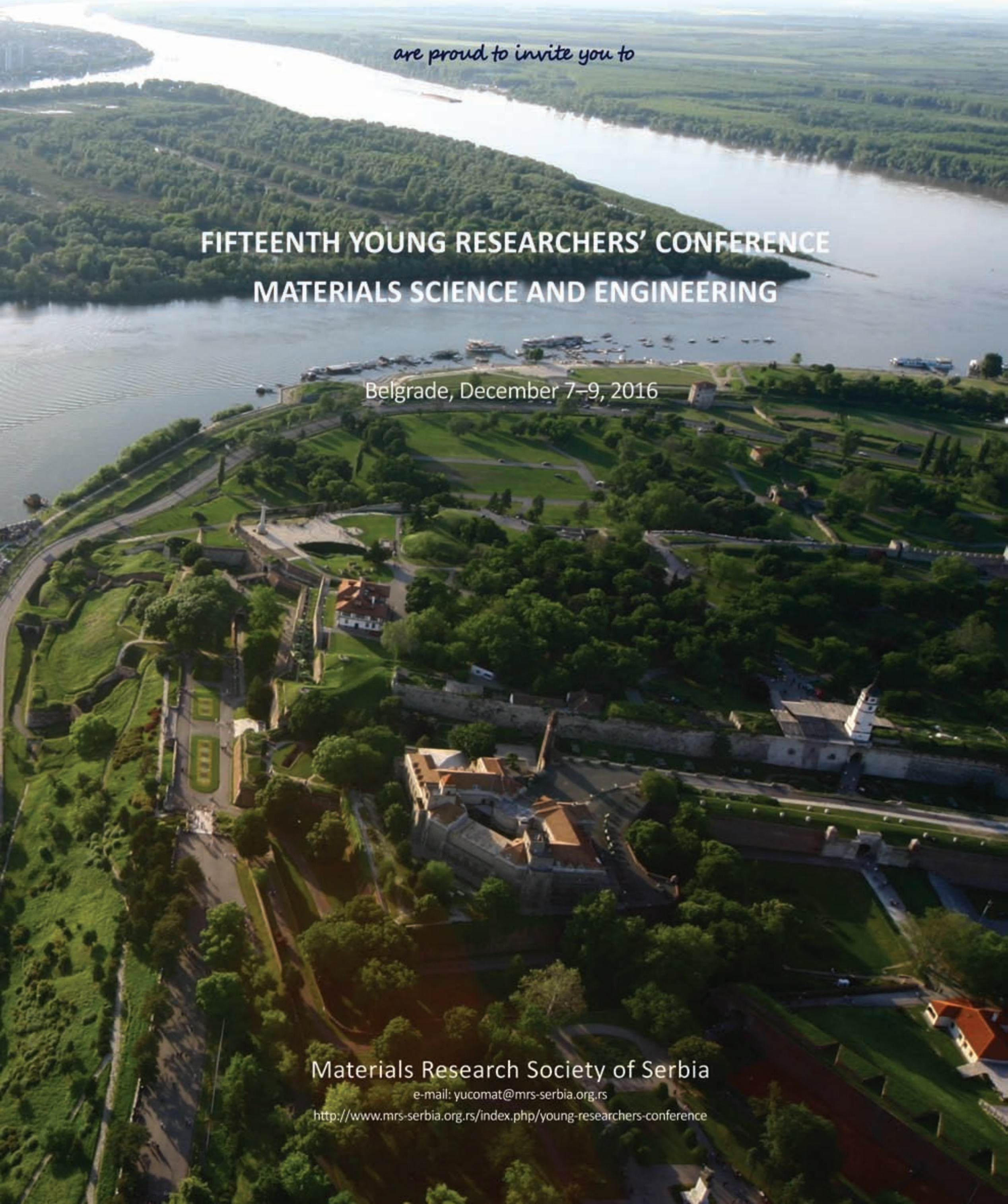

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