Programme & The Book of Abstracts

Nineteenth Annual Conference

YUCOMAT 2017

Herceg Novi, Montenegro, September 4-8, 2017

Organised by

MATERIALS RESEARCH SOCIETY OF SERBIA

endorsed by

MRS E-MRS FEMS

NINETEENTH ANNUAL CONFERENCE

YUCOMAT 2017

Hunguest Hotel Sun Resort Herceg Novi, Montenegro,
September 4-8, 2017
http://www.mrs-serbia.org.rs

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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 NINETEENTH ANNUAL CONFERENCE
YUCOMAT 2017
Programme and The Book of Abstracts

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Acknowledgments: This conference is celebrating 20 years of MRS-Serbia.

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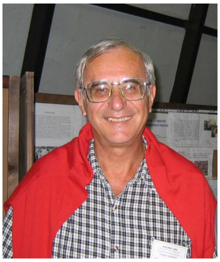
TABLE OF CONTENTS

ORAL PRESENTATIONS:

POSTER PRESENTATIONS:

WELCOME SPEECH BY THE PRESIDENT OF MRS-SERBIA:

Dear Attendees,



It is my pleasure to welcome you to the 19th YUCOMAT. Although it is 22 years now since the first YUCOMAT was held in this very coastal town of Herceg Novi, this year we celebrate the 20th anniversary of our Materials Research Society, which makes this conference as jubilar as some of the previous ones. This year, the number of plenary lecturers, all of whom are cutting-edge experts in their respective fields of materials science and engineering, is higher than ever before. Specifically, for the first time this year we exceeded the limit of 40 plenary speakers. Alongside the plenary talks, more than 100 regular talks and posters will be presented. The total of over 140 presentations will be made by participants coming from more than 30 different countries of the world. This year we also organize a premier symposium dedicated solely to the eminent scientists from the field of materials science and engineering who originate from the region of former Yugoslavia. Our desire is to bring together these remarkable researchers at one place and offer them an opportunity to meet and present on their activities with the goal of establishing or deepening scientific relations both among them and with scholars gathered around the Materials Research Society of Serbia. As of today, we intend to turn this type of symposium into a regular one and have a single day at all future conferences dedicated to it.

This year, the Society gives the third annual award for an extraordinary contribution to materials science and engineering. After Ivan Božović, the inaugural winner of this award, and Gordana Vunjak-Novaković, the winner of the last year's award, this year's award winner is Velimir-Mimo Radmilović. All three of them received formal education in Belgrade, Serbia, but matured as scientists and reached scientific fruition in the United States. Prof. Radmilović is awarded for his achievements in several areas of materials science and engineering, particularly Physical Metallurgy, Phase Transformations, Nanoscience and Nanotechnology. Moreover, he is recognized for giving a significant impetus for the growth and development of YUCOMAT into a world-renowned conference series that it is today. Thanks to his contribution, YUCOMAT has become an internationally recognized conference for which an invitation to attend and present is highly sought after.

Although YUCOMAT is officially endorsed by the world's biggest materials research societies, including MRS, E-MRS and FEMS, we could not secure a significant level of participation of their leaders this year. We will continue with our efforts to attract their eminent members in larger numbers than up to now and we look forward to their increasing participation at future events. On a more positive note, when we announced the diamond sponsorship by FEI last year, we hoped that other companies with areas of product development overlapping with the subjects of research presented at YUCOMAT would follow in similar steps and provide a valuable support for this conference series. Indeed, this has happened and the first diamond sponsor of YUCOMAT for this year is Thermo Fisher Scientific, the major biotech and lab equipment company that, as some of you may know, acquired FEI a week or so after the last year's YUCOMAT. Another diamond sponsor for this year is International Journal of Nanomedicine (Dove Medical Press, United Kingdom). This sponsorship presents an accolade for the section of the YUCOMAT program dedicated to biomedical materials, drug delivery and nanobiotechnologies. Given that nanomedicine has been one of the cores of YUCOMAT for years now, I sincerely hope that International Journal of Nanomedicine will consider the possibility of sponsoring our future events as well. Prof. Thomas Webster, the editor-in-chief of International Journal of Nanomedicine, will hold a plenary lecture on Wednesday and everybody is encouraged to attend.

Two schoolmates and two great ex-Soviet scientists, Rostislav Aleksandrovich Andrievski and Valery Vladimirovich Skorohod, who were also members of our International Advisory Board, passed away between the previous and the present YUCOMAT. They studied together at the Kiev Polytechnic Institute. Andrievski was one year older and was also one place ahead, second to none, on the list of the best students of the Institute. After graduation, they both got employed at the Institute for Problems of Materials Science of the Ukrainian Academy of Sciences and went on to make stellar scientific careers: Andrievski in the field of powder metallurgy and high-temperature materials for nuclear technologies, and Skorohod in the field of sintering theory, having become the originator of the now famous rheological theory of sintering. They both were regulars at our conferences: Andrievski at YUCOMAT and Skorohod at the earlier organized conferences on sintering. They left us in the same order: Andrievski in October 2016, right after last year's YUCOMAT, and Skorohod in June 2017. Our Society and the entire community of materials science researchers are now left without two of their giants.

In the end, a few words need be said about the socioeconomic climate in which scientists in Serbia work, earning inglorious records year after year. For example, from no place in Europe as many people per capita emigrate as from Serbia and other former Yugoslav states. Serbia, with its seven million people, the largest country that came out of the breakup of Yugoslavia, holds the first place among 138 surveyed countries in terms of the number of emigrants with higher education degrees per capita. It has been estimated that 3.5 million Serbs live abroad, as expats, whereas the emigration rate increases year after year. Only in 2014, 58.000 people permanently left Serbia, twice more than in 2007. At the same time, in 2016, Serbia had the least number of newborns in the last 100 years and its natality rate is, naturally, negative. On the opposite side of the social wheel, we witness miserably low allocations of the state budget for science – less than 15 € per capita per annum. In the absence of international collaboration, the scientific output of the country would have been catastrophic. Political nepotism has reached unsustainable proportions, while the spirit of indifference pervades the society, both in relation to the sacrifices made by the earlier generations and in relation to the eagerness to engage in bringing about a positive social change. Compared to the 1990s, when poverty and strife were more prevalent than today, the climate in Serbia is no better because, unlike in those earlier times, the keenness to expose powerful critical views seems to have completely vanished today. The silence of the public and of the intellectuals is alarming.

YUCOMAT, as ever, strives to create space for envisioning the solution to these problems. It strives to be a platform for creating cooperative bonds between scientific minds. It strives to provide a view of the frontier of research in the developed world to us, the third-world citizenry from the scientific standpoint of the day, I am afraid to say, but also put things into a fuller, healthier and more benevolent perspective to the ofttimes “spoiled” scientists from the developed world. It wishes to show that the intellectual capacity is unrelated to material wealth and that groundbreaking ideas in science often emerge from the lack, not abundance, of funds and other resources. It seeks to provide an impetus for the awakening of the local high tech economy from a deep sleep using exciting and industrially implementable basic findings, regardless of how illusory this mission may be. Finally, it strives to transmit the idea that science is more than the mere sum of its parts and that its sociopolitical, ethical and aesthetical connotations are vital to understand in order to launch a prolific scientific career, a career that must have, at all times and under all circumstances, the goal of benefitting humanity as its highest goal.

Sincerely Yours,

Dragan Uskoković,

President of MRS-Serbia

2017 MRS-SERBIA AWARD FOR A LASTING AND OUTSTANDING CONTRIBUTION TO MATERIALS SCIENCE AND ENGINEERING

We are pleased to announce that the recipient of the 2017 MRS-Serbia Award for a Lasting and Outstanding Contribution to Materials Science and Engineering is **Prof. Dr Velimir Radmilović** of Belgrade University, Lawrence-Berkeley National Laboratory USA, cor. member of Serbian Academy of Sciences and Arts (SASA). He is awarded for his achievements in several areas of Material Science and Engineering, particularly in the fields of Physical Metallurgy, Phase Transformations, Nanoscience and Nanotechnology.

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

“**T**he Executive Board of the MRS-Serbia Presidency, at their meeting on March 28, 2017, considered the submitted candidates for the MRS-Serbia’s 2017 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, 2017, and that in the stipulated period of 45 days only one candidacy was submitted, that for Prof. Dr. Velimir Radmilović, submitted by Prof. Dr. Robert Sinclair (Charles M. Pigott Professor at the Stanford University, Department of Materials Science and Engineering, CA, USA), a long-term President of the International Advisory Board and a member of the Award Committee. The candidacy was strongly supported by Prof. Dr. Ulrich Dahmen, a member of the International Advisory Board and the long-term director of the National Centre for Electron Microscopy, Lawrence Berkeley National Laboratory, as well as Prof. Dr. Hamish Fraser (Ohio State University), as well as four Members of the Presidency of the MRS Serbia (Academician Zoran Popović, Academician Zoran Petrović, Prof. Dr. Vera Dondur and Prof. Dr. Milenko Plavšić).

Having received the opinion from the Expert Committee Members, Prof. Dragan Uskokovic, Prof. Robert Sinclair, Dr. Slobodan Milonjic, Prof. Danilo Suvorov, Prof. Dejan Rakovic, Prof. Dr. Ivan Bozovic, and Prof. Dr. Gordana Vunjak-Novaković, the Executive Board of the MRS-Serbia Presidency took the decision that Prof. Dr Velimir Radmilović be granted the MRS-Serbia’s 2017 Award for a Lasting and Outstanding Contribution to Materials Science and Engineering.

Prof. Dr Velimir Radmilović's invited plenary lecture entitled *Atomistic Phenomena in Engineering Materials* will open the First Plenary Session of the 19th Materials Research Society of Serbia Annual Conference YUCOMAT 2017 on September 4, 2017.

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

MRS-Serbia
President: Dragan Uskoković
Vice-presidents: Slobodan Milonjić, Velimir Radmilović, Dejan Raković
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Conference Secretary: Aleksandra Stojičić

Conference Technical Committee
Vuk Radmilović, Sonja Jovanović, Zoran Jovanović, 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 4-8, 2017, at the Hunguest Hotel Sun Resort, in Herceg Novi, Montenegro. Participants will also be accommodated there. The conference will begin on Monday, September 4th, at 09.00 and end on Friday, September 8th, 2017, 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 3, and Monday, September 4, from 8.00 to 19.00, on Tuesday, Wednesday and Thursday 8.00-13.00 and 19.00-20.00, and on Friday from 8.00 to 12.00. At registration, the participants are requested to submit a proof of their advance registration fee payment.

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 excursion on Thursday afternoon (boat trip around Boka Kotorska Bay) will be organized again.

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: Renowned scientists from ex-Yugoslavia

Sunday, September 3 2017

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

Monday, September 4, 2017

08^{00}-19^{00}	**Registration**
09^{00}-10^{00}	**OPENING CEREMONY** - Introduction and Welcome Main Conference Hall
10^{30}-13^{00}	**First Plenary Session**, Main Conference Hall
13^{00}	**Photo Session**
15^{00}-19^{00}	**Second Plenary Session**, Main Conference Hall
19^{30}-21^{30}	**Cocktail Party**

Tuesday, September 5, 2017

09^{00}-13^{00}	**Third Plenary Session**, Main Conference Hall
15^{00}-19^{30}	**Fourth Plenary Session**, Main Conference Hall
20^{00}-22^{00}	**Poster Session I** (Symposium A and B1), Villa Mimoza

Wednesday, September 6, 2017

09^{00}-13^{00}	**Symposium F**, Main Conference Hall
15^{00}-19^{00}	**Symposium F**, Main Conference Hall
20^{00}-22^{00}	**Poster Session II** (Symposium B2 and C1), Villa Mimoza

Thursday, September 7, 2017

08^{30}-11^{00}	**Fifth Plenary Session**, Main Conference Hall
11^{30}-13^{00}	**First Oral Session**, Main Conference Hall
11^{30}-13^{00}	**Second Oral Session**, Small Conference Hall
14^{00}-19^{00}	**Boat-trip around Boka Kotorska Bay**
20^{00}-22^{00}	**Poster Session III** (Symposiums C2, D and E), Villa Mimoza

Friday, September 8, 2017

09^{00}-12^{15}	**Third Oral Session**, Main Conference Hall
09^{00}-12^{15}	**Fourth Oral Session**, Small Conference Hall
12^{30}-13^{00}	**Awards and Closing of the Conference**

OPENING CEREMONY

Monday, September 4, 2017

Main Conference Hall

09^{00}-09^{30} **Welcome Speech**
Dragan Uskoković, President of MRS-Serbia, Belgrade, Serbia
Welcome Address
Robert Sinclair, Chair of International Advisory Board
Presentation of YUCOMAT 2016 Awards
Slobodan Milonjić, Vice President of MRS-Serbia

09^{30}-10^{00} **MRS-Serbia 2017 Award for a Lasting and Outstanding Contribution to Materials Science and Engineering**
Atomistic phenomena in engineering materials
Velimir R. Radmilović
Serbian Academy of Sciences and Arts, Knez Mihailova 35, 11000, Belgrade, Serbia, and Nanotechnology and Functional Materials Center, Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11120 Belgrade, Serbia

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

FIRST PLENARY SESSION

Main Conference Hall

Session I: 10^{30}-13^{00}
Chairmen: Markus Antonietti and C. Jeffrey Brinker

10^{30}-11^{00} **Global opportunities in nanoscience and nanotechnology**
Paul S. Weiss
California NanoSystems Institute and Departments of Chemistry & Biochemistry and Materials Science & Engineering, UCLA, Los Angeles, CA 90095, USA

11^{00}-11^{30} **Analysis of next generation Quantum Materials**
David C. Bell[1], Felix VonCube[2]
[1]Harvard John A. Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, United States, [2]Hitachi High-Technologies Europe GmbH, Krefeld, Germany

11^{30}-12^{00} **Carbon nitrides as active semiconductors and supports for Artificial Photosynthesis and (Photo)Catalysis**
Markus Antonietti
Max Planck Institute of Colloids and Interfaces, Research Campus Golm, D-14424 Potsdam, Germany

12^{00}-12^{30} **Efficient CRISPR delivery via plasmid DNA (or ribonucleoprotein, RNP) packaged in mesoporous silica nanoparticles through cationic vesicle fusion**
Kim Butler[1], Rita Serda[2], Achraf Noureddine[2], Ayse Muniz[3], Darryl Sasaki[1], Oscar Negrete[1], and C. Jeffrey Brinker[1,2]
[1]Sandia National Laboratories, [2]University of New Mexico Center for Microengineered Materials and the Department of Chemical and Biological Engineering, [3]University of Michigan Biointerfaces Institute, USA

12^{30}-13^{00} **"Anything you can do I can do better" What can be done with Sonochemistry?**
Aharon Gedanken
Department of Chemistry, Bar-Ilan University, Ramat-Gan, Israel

13^{00}-13^{30} Photo session

Break: 13^{30}-15^{00}

SECOND PLENARY SESSION

Main Conference Hall

Session I: 15^{00}-16^{30}
Chairpersons: Eva Olsson and Robert Sinclair

15^{00}-15^{30} **Assessing material reactions in the environmental transmission electron microscope (TEM)**
Robert Sinclair[1], S. C. Lee[2], and A. L. Koh[3]
[1]Dept. of Materials Science & Engineering, Stanford University, Stanford, U.S.A.
[2]Dept. of Materials Science & Engineering, Stanford University, Stanford, U.S.A.,
[3]Stanford Nano Shared Facilities, Stanford University, Stanford, U.S.A.

15^{30}-16^{00} **In-situ microscopy with atomic resolution at atmospheric pressure**
Xiaoqing Pan
Department of Chemical Engineering and Materials Science, Department of Physics and Astronomy, University of California - Irvine, Irvine, California 92697, USA

16^{00}-16^{30} **In situ advanced electron microscopy of nanostructured materials for energy and quantum devices**
Eva Olsson
Department of Physics, Chalmers University of Technology, Sweden

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

Session II: 17^{00}-19^{00}
Chairmen: Knut W. Urban and Rafal E. Dunin-Borkowski

17^{00}-17^{30} **Atomic resolution imaging of materials in the chromatic and spherical aberration corrected transmission electron microscope**
Knut W. Urban and Lei Jin
Peter Gruenberg Institute, Research Center Juelich, Germany

17^{30}-18^{00} **Model-based reconstruction of magnetisation distributions in nanostructures from electron-optical phase images**
Jan Caron[1], Patrick Diehle[1], Andras Kovács[1], Jörn Ungermann[2], Rafal E. Dunin-Borkowski[1]
[1]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Forschungszentrum Jülich, 52425 Jülich, Germany, [2]Institute for Energy and Climate Research, Forschungszentrum Jülich, 52425 Jülich, Germany

18^{00}-18^{30} **Atomic resolution TEM characterization of GaSb/GaInAs and GaSb/GaInP bond interfaces for high-efficiency solar cells**
Andras Kovács[1], Felix Predan[2], Jens Ohlmann[2], David Lackner[2], Frank Dimroth[2], Rafal E. Dunin-Borkowski[1], Wolfgang Jäger[3]
[1]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Forschungszentrum Jülich, 52425 Jülich, Germany, [2]Fraunhofer Institute for Solar Energy Systems ISE, Freiburg, Germany, [3]Institute for Materials Science, Christian-Albrechts-University of Kiel, 24143 Kiel, Germany

18^{30}-19^{00} **Sub-30 meV energy resolution HR-EELS and novel HR-STEM techniques for materials science in the latest generation of Thermo Scientific Themis Z**
Dominique Delille
Materials & Structural Analysis (formerly FEI), Thermo Fisher Scientific, Achtseweg Noord 5, P.O. Box 80066, 5600KA Eindhoven, The Netherlands

19^{30}-21^{30} **Cocktail Party**

THIRD PLENARY SESSION

Tuesday, September 5, 2017

Main Conference Hall

Session I: 09^{00}-11^{00}
Chairmen: Richard W. Siegel and Vladimir Torchilin

09^{00}-09^{30} **Nanoparticles as delivery vehicles: Enabling nanocomposites and healthcare**
Richard W. Siegel
Materials Science and Engineering Department, Rensselaer Polytechnic Institute, Troy, New York 12180, USA

09^{30}-10^{00} **Multifunctional nanocarriers for drug delivery in cancer therapy**
Vladimir Torchilin
Center for Pharmaceutical Biotechnology and Nanomedicine, Northeastern University, Boston, MA 02115, USA

10^{00}-10^{30} **Targeted nanomedicines for cancer, diabetes and cardiovascular diseases: why the size matters?**
Hélder A. Santos
Division of Pharmaceutical Chemistry and Technology, Drug Research Program, Faculty of Pharmacy, and Helsinki Institute of Life Science, HiLIFE, University of Helsinki FI-00014, Helsinki, Finland

10^{30}-11^{00} **Bioinspired biomaterials for hard tissue repair and regeneration**
Anne George
Brodie Tooth Development Genetics & Regenerative Medicine Research Laboratory, Department of Oral Biology, University of Illinois at Chicago, Chicago, Illinois 60612, USA

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

Session II: 11^{30}-13^{00}
Chairmen: Horst Hahn and Hamish L. Fraser

11^{30}-12^{00} **Design of materials properties by microstructure and external fields**
Horst Hahn
Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany

12^{00}-12^{30} **Sucking the heat out of ceramic processing**
Clive A. Randall
The Pennsylvania State University, USA

12^{30}-13^{00} **Materials characterization and integrated computational materials engineering: Providing solutions for near-net shape manufacturing**
Hamish L. Fraser[1], Brian Welk[1] and Victor Samarov[2]
[1]Center for the Accelerated Maturation of Materials, The Ohio State University, Columbus, OH, [2]Synertech-PM, Garden Grove, CA, USA

Break: 13^{00}-15^{00}

FOURTH PLENARY SESSION

Main Conference Hall

Session I: 15^{00}-17^{00}
Chairmen: Martha R McCartney and David J. Smith

15^{00}-15^{30} **From low dose In-line electron holography to atomic resolution tomography**
Fu-Rong Chen[1], D. Van Dyck[2], C. Kisielowski[3]
[1]Dept. of Engineering and System Science, National Tsing Hua University, Hsin Chu, Taiwan, [2]EMAT, Department of Physics, University of Antwerp, 2020 Antwerpen, Belgium. [3]Lawrence Berkeley National Laboratory, The Molecular Foundry and Joint Center for Artificial Photosynthesis, One Cyclotron Road, Berkeley California 94720 USA

15^{30}-16^{00} **Electron holography of nanoscale electric and magnetic fields**
Martha R. McCartney, David J. Smith
Arizona State University, USA

16^{00}-16^{30} **Complex heterostructures investigated using aberration-corrected STEM**
David J. Smith and Martha R. McCartney
Department of Physics, Arizona State University, Tempe, Arizona 85287-1504, USA

16^{30}-17^{00} **Pushing the limits of electron energy loss spectroscopy for materials characterization: from phonons to core losses in real and momentum spaces**
Quentin M. Ramasse[1], Demie M. Kepaptsoglou[1], Fredrik S. Hage[1], F. Azough[2], R. Freer[2]
[1]SuperSTEM Laboratory, Daresbury, U.K., [2]School of Materials, University of Manchester, U.K.

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

Session II: 17^{30}-19^{30}
Chairmen: Laurence D. Marks and Ehrenfried Zschech

17^{30}-18^{00} **Corrosion at the nanoscale: the role of chloride**
Laurence D. Marks
Department of Materials Science and Engineering, Northwestern University, Evanston, IL 60208, USA

18^{00}-18^{30} **Sub-100nm in-situ X-ray tomography - Applications in materials science and engineering**
Ehrenfried Zschech, Jürgen Gluch, Kristina Kutukova
Fraunhofer IKTS Dresden, Germany

18^{30}-19^{00} **Atomic level characterization of novel hardening mechanisms in high-Mn-steels**
Joachim Mayer[1,2], Maryam Beigmohamadi[2], Marta Lipinska-Chwalek[1,2] and James E. Wittig[3]
[1]Central Facility for Electron Microscopy, RWTH Aachen University, Aachen, Germany, [2]Ernst Ruska Centre, Forschungszentrum Jülich, Germany, [3]Interdisciplinary Materials Science, Vanderbilt University, Nashville TN, 37235 USA

19^{00}-19^{30} **Solid-solid interface reconstruction at nominally incoherent interfaces: Ni-Al_2O_3 and Ni-YSZ**
Hadar Nahor, Hila Meltzman, and Wayne D. Kaplan
Department of Materials Science and Engineering, Technion – Israel Institute of Technology, Technion City, Haifa 32000, Israel

SYMPOSIUM F: RENOWNED SCIENTISTS FROM EX-YUGOSLAVIA

Wednesday, September 6, 2017

Main Conference Hall

Session I: 09^{00}-11^{00}
Chairmen: Radoslav R. Adžić and Nenad M. Marković

09^{00}-09^{30} **Platinum monolayer fuel cell electrocatalysts**
Radoslav R. Adžić
Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973, U.S.A.

09^{30}-10^{00} **Energy and fuels from electrochemical interfaces**
P. Papa Lopes, D. Strmcnik, V. Stamenković and Nenad M. Marković
Materials Science Division, Argonne National Laboratory, USA

10^{00}-10^{30} **Tailored materials for electrochemical applications**
Vojislav Stamenković
Argonne National Laboratory, Materials Science Division, United States

10^{30}-11^{00} **Nanostructured catalyst engineering towards efficient solar fuel production**
J. Jia[1,2], A. Jelle[1,2], G. A. Ozin[2] and Doug D. Perović[1]
[1]Department of Materials Science and Engineering, University of Toronto, Canada,
[2]Department of Chemistry, University of Toronto, Canada

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

Session II: 11^{30}-13^{00}
Chairmen: Zlatko Sitar and Gyula Eres

11^{30}-12^{00} **On the frontiers of ultra-wide bandgap semiconductors**
Zlatko Sitar
Materials Science and Engineering, North Carolina State University, USA

12^{00}-12^{30} **Exploring nanomaterials synthesis on the length scale of fundamental building blocks**
Gyula Eres
Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge TN 37831, USA

12^{30}-13^{00} **Formation mechanism of photovoltaic perovskite nanowires**
Endre Horváth[1], Massimo Spina[1], Bálint Náfrádi[1], Eric Bonvin[1], Andrzej Sienkievicz[1], Zsolt Szekrényes[2], Hajnalka Tóháti[2], Katalin Kamarás[2], Richard Gaal[3], László Forró[1]
[1]EPFL SB IPHYS LPMC, station 3, 1015, Lausanne, Switzerland, [2]Wigner Research Centre for Physics, 1525, Budapest, Hungary, [3]EPFL SB IPHYS EPSL, station 3, 1015, Lausanne, Switzerland

Break: 13^{00}-15^{00}

Session III: 15^{00}-17^{00}
Chairpersons: Tijana Rajh, Thomas J. Webster and Marija Drndić

15^{00}-15^{30} **Two decades of commercializing nanotechnology for medical devices**
Thomas J. Webster
Department of Chemical Engineering, Northeastern University, USA

15^{30}-16^{00} **TiO_2 nanocomposites for biomedical applications**
Fatima Rizvi,[1,2] Tamara Koritarov,[1,3] Nada Dimitrijević,[1] Vani Konda,[3] Marc Bissonnette,[3] Tijana Rajh[1]
[1]Center for Nanoscale Materials, Argonne National Laboratory, Lemont, Illinois, USA, [2]Department of Bioengineering, University of Illinois, Chicago, Illinois, USA, [3]Department of Medicine, The University of Chicago, Chicago, Illinois, USA

16^{00}-16^{30} **2D materials nanosculpting and bioelectronics applications**
Marija Drndić
Department of Physics and Astronomy, University of Pennsylvania, USA

16^{30}-17^{00} **Calcium phosphate as a key material for socially responsible tissue engineering**
Vuk Uskoković, Victoria M. Wu
Department of Biomedical and Pharmaceutical Sciences, Center for Targeted Drug Delivery, Chapman University, Irvine, CA 92618-1908, USA

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

Session IV: 17^{30}-19^{00}
Chairmen: Andraš Kiš and Dušan Lošić

17^{30}-18^{00} **Graphene research and development: opportunities and challenges**
Dušan Lošić, Diana Tran, Tran Thanh Tung, Md J. Nine, Shervin Kabiri, Ramesh Karunagaran, Faisal Alotaibi, Campbell Coghlan
The University of Adelaide, School of Chemical Engineering, North Eng. Building, Adelaide, 5000, SA, Australia

18^{00}-18^{30} **2D dichalcogenide electronic materials and devices**
Andraš Kiš
École Polytechnique Fédérale de Lausanne, Switzerland

18^{30}-19^{00} **Nanopores in 2D materials - opportunities and challenges**
Aleksandra Radenović
Laboratory of Nanoscale Biology, Institute of Bioengineering, School of Engineering, École Polytechnique Fédérale de Lausanne, Switzerland

FIFTH PLENARY SESSION

Thursday, September 7, 2017

Main Conference Hall

Session I: 08^{30}-11^{00}
Chairmen: Zoran V. Popović and Yimei Zhu

08^{30}-09^{00} **From MAX to MXene - From 3D to 2D**
Michel W. Barsoum
Department of Materials Science and Engineering, Drexel University, Philadelphia, PA 19104, USA

09^{00}-09^{30} **Atomically resolved interfacial coupling and polarization of ABO$_3$ heterostructures**
Yimei Zhu
Department of Condensed Mater Physics and Materials Science, Brookhaven National Laboratory, Upton, NY 11973 USA

09^{30}-10^{00} **Half-Heusler spinodal thermoelectrics with high ZT**
Peter Rogl[1], Andrij Grytsiv[1], Matthias Gürth[1], Philipp Sauerschnig[1], Jan Vrestal[2], Vitalij Romaka[3], Gerda Rogl[1], Kunio Yubuta[4], Ernst Bauer[1]
[1]Christian Doppler Laboratory for Thermoelectricity at the Institute of Materials Chemistry and Research, University of Vienna, Vienna, Austria and at the Institute of Solid State Physics, Vienna University of Technology, Vienna, Austria, [2]Department of Chemistry, Masaryk University, Kotlarska 2, Brno 61137, CR, [3]Department of Materials Science and Engineering, Lviv Polytechnic National University, 79013 Lviv, Ukraine, [4]Institute for Materials Research, Tohoku University, Katahira 2-1-1, Sendai 980-8577, Japan

10^{00}-10^{30} **Nanomagnetism: Superparamagnetism in iron - doped CeO$_2$-y nanocrystals**
Zoran V. Popović
Center for Solid State Physics and New Materials, Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

10^{30}-11^{00} **Tailoring epitaxial oxide thin film on Si(001) using pulsed-laser deposition**
Matjaž Spreitzer, Daniel Diaz, Tjaša Parkelj, Urška Gabor, Danilo Suvorov
Advanced Materials Department, Jožef Stefan Institute, Jamova 39, Ljubljana, Slovenia

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

FIRST ORAL SESSION

Main Conference Hall

Session I: 11^{30}-13^{00}

Chairpersons: Gerda Rogl and Jan Cerny

11^{30}-11^{45} **Mechanical properties of high efficiency thermoelectric materials (skutterudites, half Heusler alloys and clathrates)**
Gerda Rogl[1,2,3,4], Andriy Grytsiv[1,2,3], Ernst Bauer[1,3], Micheal Zehetbauer[4], Peter Rogl[1,2]
[1]Christian Doppler Laboratory for Thermoelectricity, [2]Institute of Materials Chemistry and Research, University of Vienna, Austria, Währingerstrasse 42, A-1090 Wien, [3]Institute of Solid State Physics, Vienna University of Technology, Austria, Wiedner Hauptstrasse, 8-10, A-1040 Wien, [4]Faculty of Physics, University of Vienna, Austria, Boltzmanngasse 5, A-1090 Wien, Austria

11^{45}-12^{00} **Plasma electrolytic oxidation of TA6V for the improvement of its surface hardness**
Marie Laveissière[1,2], Hélène Cerda[1], Jérôme Roche[2], Laurent Arurault[2]
[1]IRT Saint-Exupéry, 118 route de Narbonne – CS 44248, 31432 Toulouse cedex 4, France, [2]CIRIMAT, Université de Toulouse, CNRS, INPT, UPS, Université Toulouse III Paul Sabatier, Bât. CIRIMAT, 118 route de Narbonne, 31062 Toulouse cedex 9, France

12^{00}-12^{15} **Structural investigation of the AZ61 Magnesium alloy, in dependence of various heat treatment processes, TEM analyze**
Edlira Prespa, Jorgaq Kacani, Ylli Shehu
Polytechnic University of Tirana, Albania

12^{15}-12^{30} **Application of new modifier CaSiBa containing barium during production of low alloy steel**
Jan Černy, Pavel Ludvik, Martina Sipova, Josef Odehnal
COMTES FHT, Prumyslova 995, Dobrany, 334 41, Czech Republic

12^{30}-12^{45} **Influence of the type of substrate rotation on microstructure of magnetron sputtered nanolayered TiAlN/TiSiN coatings**
Aleksandar Miletić[1], Peter Panjan[2], Miha Čekada[2], Lazar Kovačević[1], Pal Terek[1], Branko Škorić[1], Goran Dražič[3], Janez Kovač[2]
[1]Faculty of Technical Sciences, University of Novi Sad, Novi Sad, Serbia, [2]Jožef Stefan Institute, Ljubljana, Slovenia, [3]National Institute of Chemistry, Ljubljana, Slovenia

12^{45}-13^{00} **Synthesis and thermal stability of immiscible metal (Au–Rh, Au–Ir, Au–Ir–Rh and Pd-Rh) nanoalloys**
Yury Shubin, Pavel Plyusnin, Sergey Korenev, Aleksey Vedyagin
[1]Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk, Russia, [2]Boreskov Institute of Catalysis SB RAS, Novosibirsk, Russia

SECOND ORAL SESSION

Small Conference Hall

Session I: 11^{30}-13^{00}
Chairmen: Branko Matović and Błażej Scheibe

11^{30}-11^{45} **Synthesis, processing, thermal and luminescence properties of Eu^{3+} -doped Gd_2O_3 powders**
Branko Matović[1], Jelena Maletaskić[1], Marija Prekajski Đorđević[1], Katsumi Yoshida[2], Toyohiko Yano[2], Marko Nikolić[3], Branimir Jelenković[3]
[1]Centre of Excellence-CextremeLab Vinca, Institute for Nuclear Sciences, University of Belgrade, Belgrade, Serbia, [2]Laboratory for Advanced Nuclear Energy, Institute of Innovative Research, Tokyo Institute of Technology, 2-12-1, Ookayama, Meguro-ku, Tokyo, 152-8550 Japan, [3]Institute for Physics, University of Belgrade

11^{45}-12^{00} **Interrelations between positive and negative coercive fields of ferroelectric domains measured by variable amplitude cycling**
Mikhail V. Katkov[1,2] and Yuriy V. Pershin[3,1]
[1]Nikolaev Institute of Inorganic Chemistry SB RAS, Novosibirsk 630090, Russia, [2]Institute of Systems Science, Durban University of Technology, P.O. Box 1334, Durban 4000, South Africa, [3]Department of Physics and Astronomy, University of South Carolina, Columbia, SC 29208 USA

12^{00}-12^{15} **Synthesis and characterization of $Li_2FeP_2O_7$ cathode material**
Dragana Jugović[1], Miloš Milović[1], Miodrag Mitrić[2], Nikola Cvjetićanin[3], Srečo Škapin[4], Dragan Uskoković[1]
[1]Institute of Technical Sciences of SASA, Belgrade, Serbia, [2]Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia, [3]Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia, [4]Jožef Štefan Institute, Jamova 39, SI-1000 Ljubljana, Slovenia

12^{15}-12^{30} **Preparation, modification and application of multi-layered MXene structures in gas sensors**

Błażej Scheibe[1], Katarzyna Dunst[2], Marcin Jarek[1], Barbara Peplińska[1], Piotr Jasiński[2], Stefan Jurga[1]
[1]NanoBioMedical Centre Adam Mickiewicz University in Poznań, [2]Faculty of Electronics, Telecommunications and Informatics, Gdańsk University of Technology, Poland

12^{30}-12^{45} **Tuning electronic properties of MoS_2 by doping nonisovalent niobium and rhenium ions**

Alexandra Yu. Ledneva, Svetlana A. Dalmatova, Anastasiya D. Fedorenko, Lev N. Mazalov, Vladimir E. Fedorov
Nikolaev Institute of Inorganic Chemistry SB RAS, Russia

12^{45}-13^{00} **Enhanced natural sunlight- and artificial UV-driven photocatalytic activity of mechanically activated ZnO/SnO_2 composite**

Smilja Marković[1], Ana Stanković[1], Jasmina Dostanić[2], Lidija Mančić[1], Srečo Davor Škapin[3], Dragan Uskoković[1]
[1]Institute of Technical Sciences of SASA, Knez Mihailova 35/IV, 11000 Belgrade, Serbia, [2]University of Belgrade, IChTM Center for Catalysis, Belgrade, Serbia, [3]Jožef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia

THIRD ORAL SESSION

Friday, September 8, 2017

Main Conference Hall

Session I: 09^{00}-10^{30}
Chairpersons: Nenad L. Ignjatović and Irena Nikolić

09^{00}-09^{15} **Highly selective anticancer activity of core shell particles based on hydroxyapatite, chitosan lactate and different androstane derivatives**
Nenad L. Ignjatović[1], Katarina M. Penov-Gaši[2], Jovana J. Ajduković[2], Marija Sakač[2], Ivana Kuzminac[2], Vesna V. Kojić[3], Smilja Marković[1], Dragan P. Uskoković[1]
[1]Institute of Technical Sciences of the Serbian Academy of Science and Arts, Knez Mihailova 35/IV, P.O. Box 377, 11000 Belgrade, Serbia, [2]University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia, [3]Oncology Institute of Vojvodina, Put Dr Goldmana 4, 21204 Sremska Kamenica, Serbia

09^{15}-09^{30} **The atomic-scale defects at the surface of MgO particles and their antibacterial applications**
Nemanja Aničić, Marija Vukomanović, Danilo Suvorov
Advanced Materials Department, Jozef Stefan Institute, Jamova 39 Ljubljana, Slovenia

09^{30}-09^{45} **Design and evaluation of biocompatible 90Y-labeled phosphate-coated MNPs for possible applications in cancer therapy**
Magdalena Radović, Marija Mirković, Drina Janković, Aleksandar Vukadinović, Marko Perić, Dragana Stanković, Đorđe Petrović, Sanja Vranješ-Đurić
University of Belgrade, Vinča Institute of Nuclear Sciences, Laboratory for radioisotopes, P. O. Box 522, 11001 Belgrade, Serbia

09^{45}-10^{00} **Hierarchical self-assembly of highly water-soluble fullerene derivatives**
Ilija Rašović and Kyriakos Porfyrakis
Department of Materials, University of Oxford, UK

10^{00}-10^{15} **Networks of welded silver nanowires as transparent electrodes**
Vuk V. Radmilović[1], Peter Ercius[2], Colin Ophus[3], Erdmann Spiecker[4], Velimir R. Radmilović[5]
[1]Innovation Center, Faculty of Technology and Metallurgy, University of Belgrade, Serbia, [2]National Center for Electron Microscopy, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, USA, [3]National Center for Electron Microscopy, Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, USA, [4]Center for Nanoanalysis and Electron Microscopy, Friedrich Alexander University, Erlangen, Germany, [5]Serbian Academy of Sciences and Arts, Belgrade, Serbia

10^{15}-10^{30} **Properties of organic conjugated molecules sensitized by fullerenes**
Svetlana Vladimirovna Likhomanova[1], Natalia Vladimirovna Kamanina[1,2]
[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,197376, Russia

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

Session II: 11^{00}-12^{15}
Chairmen: Satoshi Ohara and Wilfried Gille

11^{00}-11^{15} **Organic-ligand-assisted hydrothermal synthesis of tailor-made ceramic nanocrystals towards bio-medical applications**
Satoshi Ohara[1], Kosuke Nozaki[2], Akiko Nagai[2], and Kimihiro Yamashita[2]
[1]Joining and Welding Research Institute, Osaka University, [2]Institute of Biomaterials and Bioengineering, Tokyo Medical and Dental University, Japan

11^{15}-11^{30} **Small-angle scattering of non-convex nanoparticles: The case of a cube, possessing a rectangular indent**
Wilfried Gille
Formerly of Martin-Luther-University Halle-Wittenberg, Institute of Physics, SAS Laboratory, Germany

11^{30}-11^{45} **Au hollow cylindrical nanostructures as optical tunable nanoresonators**
Ana Conde-Rubio[1,2], Francesc Pérez-Murano[3], Xavier Batlle[1,2], Amilcar Labarta[1,2]
[1]Department de Física de la Matèria Condensada, Universitat de Barcelona, Barcelona, Spain, [2]Institut de Nanociència i Nanotecnologia(IN2UB), Universitat de Barcelona, [3]Instituto de Microelectrónica de Barcelona (IMB-CNM, CSIC) UAB, 08193 Bellaterra, Barcelona, Spain

11^{45}-12^{00} **Process development for reproducible synthesis of magnetic eco-friendly adsorbent**

Doina Hritcu, Alina Ibanescu, Marcel I. Popa
Faculty of Chemical Engineering and Environmental Protection, “Gheorghe Asachi” Technical University of Iasi, Romania

12^{00}-12^{15} **The slag based adsorbents for Cu^{2+} removal from aquatic solutions**

Irena Nikolić[1], Dijana Đurović[2], Ivana Milašević[3], Smilja Marković[4], Vuk V. Radmilović[5], Velimir R. Radmilović[6]
[1]University of Montenegro, Faculty of Metallurgy and Technology, Podgorica, Montenegro, [2]Institut of Public Health of Montenegro, Podgorica, Montenegro, [3]Centre of Excellence in Bioinformatics, Faculty of Electrical Engineering, University of Montenegro, Podgorica, Montenegro, [4]Institute of Technical Sciences of SASA, Belgrade, Serbia, [5]Innovation center, University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia, [6] Serbian Academy of Sciences and Arts, Belgrade, Serbia

FOURTH ORAL SESSION

Small Conference Hall

Session I: 09^{00}-10^{30}
Chairpersons: Julija R. Šćepanović and Marko Radović

09^{00}-09^{15} **Particle morphology effects in random sequential adsorption**

Ljupka Budinski Petković[1], Ivana Lončarević[1], Dijana Dujak[2], Aleksandar Karac[3], Julija R Šćepanović[4], Zorica M Jakšić[4], Slobodan B Vrhovac[4]
[1]Faculty of Engineering, Trg D. Obradovica 6, Novi Sad, 21000 Serbia, [2]Faculty of Metallurgy and Materials, University of Zenica, Zenica, Bosnia and Herzegovina, [3]Polytechnic Faculty, University of Zenica, Zenica, Bosnia and Herzegovina, [4]Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, Zemun 11080, Belgrade, Serbia

09^{15}-09^{30} **Inkjet printing of TiO_2 nanoparticles on flexible substrates**

Slavica M. Savić[1], Sanja Kojić[2], Jaroslav Katona[3], Jelena Vukmirović[3], Georges Dubourg[1], George Niarchos[1], Marko Radović[1]
[1]Biosense Institute, Research Institute for Information Technologies in Biosystems, Novi Sad, Serbia, [2]Faculty of Technical Sciences, University of Novi Sad, Novi Sad, Serbia, [3]Faculty of Technology, University of Novi Sad, Novi Sad, Serbia

09^{30}-09^{45} **Photocatalytic hollow TiO_2 and ZnO nanospheres prepared by atomic layer deposition**

László Péter Bakos[1], Nóra Justh[1], Klára Hernádi[2], Gabriella Kiss[2], Balázs Réti[2], Zoltán Erdélyi[3], Bence Parditka[3] and Imre Miklós Szilágyi[1]

[1]Department of Inorganic and Analytical Chemistry, Budapest University of Technology and Economics, H-1111 Budapest, Hungary, [2]Department of Applied and Environmental Chemistry, University of Szeged, H-6720 Szeged, Hungary, [3]Department of Solid State Physics, University of Debrecen, H-4026 Debrecen, Hungary

09^{45}-10^{00} **Preparation of iron tungstate ($FeWO_4$) nanosheets by hydrothermal method**

Teodóra Nagyné Kovács[1,*], György Pokol[1,2], Fanni Gáber[1], Dávidné Nagy[3], Tamás Igricz[4], István Endre Lukács[5], Zsolt Fogarassy[5], Katalin Balázsi[5], Imre M. Szilágyi[1]

[1]Department of Inorganic and Analytical Chemistry, Budapest University of Technology and Economics, Műegyetem rakpart 3., Budapest, H-1111, Hungary, [2]Research Centre for Natural Sciences, Hungarian Academy of Sciences, Magyar tudósok körútja 2., Budapest, H-1117, Hungary, [3]Institute for Materials and Processes, School of Engineering, The University of Edinburgh, The King's Buildings, Mayfield Road, Edinburgh, EH9 3JL, United Kingdom, [4]Department of Organic Chemistry and Technology, Budapest University of Technology and Economics, H–1111 Budapest, Budafoki út 8. Hungary; [5]Research Institute for Technical Physics and Materials Science, Hungarian Academy of Sciences, Konkoly-Thege út 29-33., Budapest, H-1121 Hungary

10^{00}-10^{15} **Preparation and investigation of the photocatalytic properties of core/shell nanocomposites**

Orsolya Kéri[1], Eszter Kocsis[1], Lenke Kócs[2], Zoltán Hórvölgyi[2], Levente Kárpáti[2], Bence Parditka[3], Zoltán Erdélyi[3], Imre Miklós Szilágyi[1]

[1]Budapest University of Technology and Economics, Department of Inorganic and Analytical Chemistry, [2]Budapest University of Technology and Economics, Department of Physical Chemistry and Materials Science, [3]University of Debrecen, Department of Solid State Physics, Hungary

10^{15}-10^{30} **Reductive properties of nanocrystalline Al-modified cobalt oxides: in situ XRD investigation**
Svetlana Cherepanova[1,2], Olga Bulavchenko[1,2], Irina Simentsova[1]
[1]Boreskov Institute of Catalysis, Lavrentieva prospect 5, Novosibirsk, 630090, Russia, [2]Novosibirsk State University, Pirogova street 2, Novosibirsk, 630090, Russia

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

Session II: 11^{00}-12^{15}
Chairmen: Waldemar Swiderski and Alexander Kurbakov

11^{00}-11^{15} **Non-destructive testing of cover made of CFRP after ballistic impacts by IR thermography methods**
Waldemar Swiderski
Military Institute of Armament Technology, Poland

11^{15}-11^{30} **Ductile/brittle polymer system modified with carbon nanoplatelets: Effect of components coupling**
Ivan Kelnar, Jaroslav Kratochvíl
Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovsky Sq. 2, 162 06 Prague, Czech Republic

11^{30}-11^{45} **Neutron and synchrotron diffraction studies of low dimensional frustrated magnets with unique magnetic, electrical and redox properties**
Alexander Kurbakov[1,2], Artem Korshunov[1,2], Mariia Kuchugura[1,2], Stanislav Podchezertsev[1], Juan Rodriguez-Carvajal[3]
[1]Petersburg Nuclear Physics Institute, NRC Kurchatov Institute, 188300, Gatchina, Russia, [2]St.Petersburg State University, Faculty of Physics, 198504, St. Petersburg, Russia, [3]Institut Laue Langevin – CS 20156 - 38042 Grenoble, France

11^{45}-12^{00} **The study of the correlation between surface chemistry and charge storage properties of graphene oxide**
Zoran Jovanović[1], Danica Bajuk-Bogdanović[2], Sonja Jovanović[1], Željko Mravik[2], Ivanka Holclajtner-Antunović[2], Milica Vujković[2]
[1]Laboratory of Physics, Vinča Institute of Nuclear Sciences, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia, [2]Faculty of Physical Chemistry, University of Belgrade, P.O. Box 47, 11158 Belgrade, Serbia

12^{00}-12^{15} **Influence of zinc doping on the magnetic properties of cobalt ferrite nanoparticles**

Sonja Jovanović[1], Bojana Nedić-Vasiljević[2], Danica Bajuk-Bogdanović[2], Davide Peddis[3]

[1]Laboratory of Physics, Vinca Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia, [2]Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia, [3]nM2-Lab, Istituto di Struttura della Materia, CNR, Monterotondo Scalo (Roma) 00015, Italy

$\mathbf{12^{30}}$-$\mathbf{13^{00}}$ CLOSING CEREMONY in Main Hall

POSTER SESSION I

Tuesday, September 5, 2017, 20^{00}-22^{00}

SYMPOSIUM A: ADVANCED METHODS IN SYNTHESIS AND PROCESSING OF MATERIALS

P.S.A.1. **Preparation and properties of photocatalyst in TiO_2-ZnO system**
Anita Letlena, Jānis Grabis, Aija Krūmiņa
Riga Technical University, Faculty of Material Science and Applied Chemistry, Institute of Inorganic Chemistry, Latvia

P.S.A.2. **Modified TiO_2 thin films prepared by spray pyrolysis deposition and their photocatalytic activity**
Laura Rozenberga-Voska, Jānis Grabis
Institute of Inorganic Chemistry, Faculty of Material Science and Applied Chemistry, Riga Technical University, Latvia

P.S.A.3. **Nanobanksia - novel hybrid inorganic/organic nanomaterial**
Aleš Mrzel, Damjan Vengust, Mojca Vilfan
Jozef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia

P.S.A.4. **Leaching of trace elements from packaging material into canned meat products**
Branislav Stojanović[1], Ljubica Radović[2], Tatjana Šolević Knudsen[3], Branimir Jovančićević[4], Tanja Petrović[5], Steva Lević[5] and Vesna Antić[5]
[1]Ministry of Defence-Republic of Serbia, Belgrade, Serbia, [2]Military Technical Institute, Belgrade, Serbia, [3]Institute of Chemistry, Technology and Metallurgy, Belgrade, Serbia, [4]University of Belgrade-Faculty of Chemistry, Belgrade, Serbia, [5]University of Belgrade-Faculty of Agriculture, Zemun, Serbia

P.S.A.5. **Characterization of pressureless sintered $MgO-Al_2O_3-SiO_2-TeO_2$ system**
Nina Obradović[1], Nataša Đorđević[2], Darko Kosanović[1], Suzana Filipović[1], Martin Kachlik[3], Karel Maca[3], Dragan Olćan[4], Antonije Đorđević[4,5], Vladimir Pavlović[1]
[1]Institute of Technical Sciences of SASA, Knez Mihailova 35/IV, 11000 Belgrade, Serbia, [2]Institute for Technology of Nuclear and Other Mineral Raw Materials, Bulevar Franse d'Eperea 86, 11000 Belgrade, Serbia, [3]CEITEC BUT, Brno University of Technology, 61600 Brno, Czech Republic, [4]School of Electrical Engineering, University of Belgrade, Bulevar kralja Aleksandra 73, 11000 Belgrade, Serbia, [5]Serbian Academy of Sciences and Arts, Knez Mihailova 35, 11000 Belgrade, Serbia

P.S.A.6. **Temperature responsive hydrogels based on ethylene glycol propylene glycol “block” units with VPTT close to human body temperature**
Edin Suljovrujić, Maja Mićić, Zorana Rogić Miladinović, Dejan Miličević
Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia

P.S.A.7. **Composition of red mud and/or metakaolin-based modified geopolymers**
Mira Vukčević[1], Ivana Bošković[1], Snežana Nenadović[2], Miljana Mirković[2], Bojan Čalija[3], Vladimir Pavlović[4], and Ljiljana Kljajević[2]
[1]Faculty of Metallurgy and Technology, University of Montenegro, [2]Laboratory for Materials Sciences, Institute of Nuclear Sciences Vinča, University of Belgrade, Serbia, [3]Department of Pharmaceutical Technology, Faculty of Pharmacy, University of Belgrade, Serbia, [4]Institute of Technical Sciences of the Serbian Academy of Sciences and Arts, University of Belgrade, Serbia

P.S.A.8. **Fabrication and characterization of Al-5 wt.% Si matrix composites reinforced with various boride particles**
Duygu Ağaoğulları, Sıddıka Mertdinç, Emre Tekoğlu, M. Lütfi Öveçoğlu
Istanbul Technical University, Chemical and Metallurgical Engineering Faculty, Metallurgical and Materials Engineering Department, Particulate Materials Laboratories (PML), 34469 Maslak, Istanbul, Turkey

P.S.A.9. **Combustion synthesis of yttrium aluminum perovskites doped by rare earth ions**
Daniel Michalik[1], Krzysztof Strzech[1], Radoslaw Lisiecki[2], Tomasz Pawlik[1], Malgorzata Sopicka Lizer[1]
[1]Silesian University of Technology, Department of Materials Science, Krasinskiego 8, 40-019 Katowice, Poland, [2]Institute of Low Temperature and Structure Research, Okolna 2, 50-422 Wroclaw, Poland

P.S.A.10. **Modification of poly(ethylene terephthalate) by blending with polyamide-6 utilizing reactive compatibilization**
Seung Yong Shin[1], Kwan Han Yoon[2], Byung Gil Min[3]
[1&2]Dept. of Materials Design and Engineering, Kumoh National Institute of Technology, Korea, [3]Dept. of Chemical Engineering, Kumoh National Institute of Technology, Korea

P.S.A.11. **Thermal and mechanical properties of poly(ethylene terephthalate) copolymer containing bis(dimethyl-2-hydroxyethyl) tetraoxaspiro undecane**
Seung Ho Jeong[1], Byung Gil Min[2], Kwan Han Yoon[1]
[1]Department of Chemical Engineering, and [2]Department of Material Design Engineering, Kumoh National Institute of Technology, Gumi, 730-701, Korea

SYMPOSIUM B: ADVANCED MATERIALS FOR HIGH-TECHNOLOGY APPLICATIONS – SESSION 1

P.S.B.1. **The influence of changes in Ca/Y concentration ratio on the spectroscopic properties of europium doped $Ca_9Y(PO_4)_7$ phosphor for white light emitting diodes**
Natalia Gorecka, K. Szczodrowski, A. Lazarowska, J. Barzowska, M. Grinberg
Institute of Experimental Physics, Faculty of Mathematics, Physics and Informatics, University of Gdansk, Wita Stwosza 57, 80-308 Gdansk, Poland

P.S.B.2. **Spectroscopic properties of Eu^{2+} and Eu^{3+} doped barium potassium phosphate**
Anna Baran[1], Sebastian Mahlik[1], Marek Grinberg[1], Adam Watras[2], Robert Pazik[2], Przemyslaw Deren[2]
[1]Institute of Experimental Physics, Faculty of Mathematics, Physics and Informatics, University of Gdansk, Wita Stwosza 57, 80-308 Gdansk, Poland, [2]Institute of Low Temperature and Structure Research, Polish Academy of Sciences, 2 Okólna Street, 50-422 Wroclaw, Poland

P.S.B.3. **Effect of external influences on Fe- Cr - based alloys studied by positron annihilation spectroscopy**
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.4. **The optimization of EVA monolith synthesis for effective immobilization of Candida rugosa lipase**
Zorica Veličić[1], Nataša Tomić[2], Nevena Prlainović[2], Jelena Rusmirović[2], Aleksandar D. Marinković[3], Milka Vidović[1]
[1]Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 4, 11000, Serbia, [2]Innovation Center of the Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11120 Belgrade, Serbia, [3]Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11120 Belgrade, Serbia

P.S.B.5. **Transport properties of Ar^+ in Ar/CF_4 mixtures for technological applications**
Željka Nikitović, Zoran Raspopović and Vladimir Stojanović
Institute of Physics University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

P.S.B.6. **Optimization of magnetoimpedance sensing properties of FeCuNbSiB amorphous microwires**
Nebojša Mitrović, Jelena Orelj, Siniša Ranđić, Slobodan Đukić
Faculty of Technical Sciences Čačak, University of Kragujevac, Serbia

P.S.B.7. Improvement of cup anemometer class by bearing design

Miodrag Zlatanović and Ivan Popović
School of Electrical Engineering, University of Belgrade, Serbia

POSTER SESSION II

Wednesday, September 6, 2017, 20^{00}-22^{00}

SYMPOSIUM B: ADVANCED MATERIALS FOR HIGH-TECHNOLOGY APPLICATIONS – SESSION 2

P.S.B.8. **Determination of the elastic modulus of partially intercalated and exfoliated polymer-clay nanocomposites using numerical homogenization techniques**
Youcef Djebara[1], Salah Madani[1], Toufik Kanit[2]
[1]Laboratory of Mechanical Structures and Materials, University of Batna 2, Algeria, [2]Laboratory of Mechanics of Lille, University of Lille 1, France

P.S.B.9. **Production of 99Mo/99mTc generators - Advantages of dry column**
Đorđe Petrović, Marko Perić, Drina Janković, Aleksandar Vukadinović, Dragana Stanković, Marija Mirković, Magdalena Radović, Sanja Vranješ-Đurić
University of Belgrade, Vinča Institute of Nuclear Sciences, Laboratory for radioisotopes, P. O. Box 522, 11001 Belgrade, Serbia

P.S.B.10. **High-energy spectroscopy of YbM_2P_2 compounds**
Ivan Shcherba[1,2], Henrik Noga[1], Viktor Antonov[3], Dragan Uskoković[4], Maria Kovalska[2], Bohdan Jatcyk[5]
[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 Physics of Metals, NASU, Kyiv, Ukraine, [4]Institute of Technical Sciences of SASA, Belgrade, Serbia, 5Lviv National University of Veterinary Medicine and Biotechnologies, Lviv, Ukraine

P.S.B.11. **Influence of electrode thickness on the electrochemical properties of activated ion-track carbon supercapacitors**
Petar Laušević[1,2], Milica Marčeta Kaninski[1], Vladimir Nikolić[1], Pavel Apel[3], Maria Eugenia Toimil-Molares[4] and Zoran Laušević[1]
[1]Laboratory of physical chemistry, Vinča institute of nuclear sciences, University of Belgrade, PO Box 522, 11001 Belgrade, Serbia, [2]School of Electrical Engineering, University of Belgrade, Bulevar kralja Aleksandra 73, 11120 Belgrade, Serbia, [3]Flerov laboratory of nuclear reactions, Joint institute for nuclear research, 141980 Dubna, Russia, [4]GSI Helmholtzzentrum für Schwerionenforschung, 64291 Darmstadt, Germany

P.S.B.12. **Temperature dependence of relaxation times of quasiparticles in 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.13. **Crystal structure and magnetic properties of $Bi_{1-x}Ae_xFe_{1-x}Ti_xO_3$ (Ae=Ca, Sr, Ba) multiferroics**
Uladzimir Khomchanka and José António Paixão
CFisUC, Department of Physics, University of Coimbra, P-3004-516 Coimbra, Portugal

P.S.B.14. **The fabrication of tubular spinel cobalt manganese oxide by single-spinneret electrospinning as a high-performance electrode for aqueous supercapacitors**
Daniel M. Mijailović, Vesna J. Radojević, Dušica B. Stojanović, Đorđe T. Janaćković, Petar S. Uskoković
University of Belgrade, Faculty of Technology and Metallurgy; Serbia

SYMPOSIUM C: NANOSTRUCTURED MATERIALS – SESSION 1

P.S.C.1. **Effect of W-doped TiO_2 nanopowders on photocatalytic degradation of selected psychoactive drugs**

Nina Finčur[1], Maja Šćepanović[2], Mirjana Grujić-Brojčin[2], Aleksandar Golubović[2], 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 Belgrade, Institute of Physics, Center for Solid State Physics and New Materials, Pregrevica 118, 11080 Belgrade, Serbia

P.S.C.2. **Activity of pure ZnO and ZnO/MWCNTs nanoparticles in degradation of clomazone under different type of irradiation**

Vesna Despotović[1], Nina Finčur[1], Goran Bošković[2], Sanja Panić[2], Biljana Abramović[1]

[1]University of Novi Sad, Department of Chemistry, Biochemistry and Environmental Protection, Faculty of Sciences, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia, [2]University of Novi Sad, Faculty of Technology, Bulevar Cara Lazara 1, Novi Sad, Serbia

P.S.C.3. **In-situ study of the oxygen-induced transformation of pyrochlore $Ce_2Zr_2O_{7+x}$ to the kK-$Ce_2Zr_2O_8$ phase**

Igor Đerđ[1], Sven Urban[2], Paolo Dolcet[3], Limei Chen[4], Maren Möller[2], Silvia Gross[3], Peter J. Klar[4], Bernd Smarsly[2], Herbert Over[2]

[1]Department of Chemistry, Josip Juraj Strossmayer University of Osijek, Cara Hadrijana 8/A, 31000 Osijek, Croatia, [2]Physikalisch-Chemisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 17, 35392 Gießen, Germany, [3]Dipartimento di Scienze Chimiche, Università degli Studi di Padova via Francesco Marzolo, 1, I-35131 Padova, Italy, [4]I. Physikalisches Institut, Justus Liebig University, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

P.S.C.4. **One-step production of nanoalloys in Pt-Co, Pt-Fe, Pt-Ni systems**

Evgeny Y. Filatov, Andrey V. Zadesenets, Sergey V. Korenev

[1]Nikolaev Institute of Inorganic Chemistry of Siberian Branch of the Russian Academy of Sciences, Akademika Lavrenteva ave., 3, Novosibirsk, 630090, Russia, [2]Novosibirsk State University, Pirogova str., 2, Novosibirsk, 630090, Russia

P.S.C.5. **Liquid phase sodium intercalation into layered transition metal chalcogenides**

Pavel A. Poltarak, Sofia B. Artemkina, Vladimir E. Fedorov

Nikolaev Institute of Inorganic Chemistry, Russia

P.S.C.6. **Temperature dependence of morphology and size of ZrS_3 and TiS_3 particles in colloidal dispersions**

Anastasiia A. Poltarak, Pavel A. Poltarak, Mariia N. Kozlova, Sofia B. Artemkina, Vladimir E. Fedorov
Nikolaev Institute of Inorganic Chemistry, Russia

P.S. C.7. **Oxidative longitudinal unzipping of short MWCNTs toward graphene nanoribbons**

Igor Medić[1], Sanja Panić[2], Elvira Đurđić[3], Danica Jović[1], Goran Bošković[2], Željka Cvejić[3], Srđan Rakić[3], Aleksandar Đorđević[1]
[1]Department of Chemistry, Biochemistry and Environmental Protection, Faculty of Sciences, University of Novi Sad, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia, [2]Faculty of Technology, University of Novi Sad, Bulevar Cara Lazara 1, 21000 Novi Sad, Serbia, [3]Department of Physics, Faculty of Sciences, University of Novi Sad, Trg Dositeja Obradovića 4, 21000 Novi Sad, Serbia

P.S.C.8. **Selectivity manipulation of ultrathin film-structure optical characteristics**

Jovan P. Šetrajčić[1], Igor J. Šetrajčić[1], Ana J. Šetrajčić–Tomić[2], Siniša M. Vučenović[3], and Stevo K. Jaćimovski[4]
[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, [4]Academy of Criminalistic and Police Studies, Zemun – Belgrade, Serbia

P.S.C.9. **Accelerated service life test of electrodeposited NiSn coatings as bifunctional hydrogen and oxygen evolution catalysts for alkaline water electrolysis**

Ljiljana Gajić-Krstajić[1], Vladimir Jović[2], Borka Jović[2], Uroš Lačnjevac[2], Nedeljko Krstajić[3], Piotr Zabinski[4], Nevenka Elezović[2]
[1]Institute of Technical Sciences SASA, Knez Mihajlova 35, 11000 Belgrade, Serbia, [2]Institute for Multidisciplinary Research University of Belgrade, P.O. Box 33, 11030 Belgrade, Serbia, [3]Faculty of Technology and Metallurgy University of Belgrade, Karnegijeva 4, 11000 Belgrade, Serbia, [4]AGH University of Science and Technology, Faculty of Non-Ferrous Metals, Al. Mickiewicza 30,30-059 Krakow, Poland

P.S.C.10. **Zero-dimensional hexagonal stanene nanostructures in a magnetic field**

Dušan Z. Jakovljević[1], Milan Ž. Tadić[1], Marko M. Grujić[1], Vladimir V. Arsoski[1], François M. Peeters[2]
[1]School of Electrical Engineering, Unversity of Belgrade, P.O. Box 3554, 11120 Belgrade, Serbia, [2]Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerp, Belgium

P.S.C.11. **Three novel bis-phosphonate-coated MNPs labeled with 99mTc as multifunctional agents for possible use in medicine**

Marija Mirković, Magdalena Radović, Drina Janković, Aleksandar Vukadinović, Marko Perić, Dragana Stanković, Đorđe Petrović, Sanja Vranješ-Đurić
University of Belgrade, Vinča Institute of Nuclear Sciences, Laboratory for radioisotopes, P. O. Box 522, 11001 Belgrade, Serbia

P.S.C.12. **Spectral analysis of the ordering effect of starch coated magnetite nano-particles**

Marko Perić, Drina Janković, Aleksandar Vukadinović, Dragana Stanković, Đorđe Petrović, Marija Mirković, Magdalena Radović, Sanja Vranješ-Đurić
University of Belgrade, Vinča Institute of Nuclear Sciences, Laboratory for radioisotopes, P. O. Box 522, 11001 Belgrade, Serbia

POSTER SESSION III

Thursday, September 7, 2017, 20^{00}-22^{00}

SYMPOSIUM C: NANOSTRUCTURED MATERIALS – SESSION 2

P.S.C.13. **Electrospun PMMA nanofibers doped with CdSe/ZnS core shell quantum dots**
Rouaida M. Abozaid[1], Dušica B. Stojanović[1], Anđela Radisavljević[1], Dragutin M. Sević[2], Maja S. Rabasović[2], Petar S. Uskoković[1], Vesna Radojević[1]
[1]University of Belgrade, Faculty of Technology and Metallurgy, Belgrade,
[2]University of Belgrade, Institute of Physics, Zemun, Serbia

P.S.C.14. **Formation of nanocrystalline 9R silicon hexagonal phase under multi-ion implantation into Si and SiO_2/Si substrates**
David Tetelbaum, Dmitry Korolev, Alena Nikolskaya, Alexey Belov, Alexey Mikhaylov, Nikolay Krivulin, Dmitry Pavlov
Lobachevsky University, Nizhny Novgorod, Russia

P.S.C.15. **Enhancing Pt catalytic properties by addition of Au: Could less be more?**
Mila N. Krstajić Pajić[1], Sanja I. Stevanović[1], Vuk V. Radmilović[2], Nevenka R. Elezović[3], Piotr Zabinski[4], Nedeljko V. Krstajić[5], Velimir R. Radmilović[5,6], Snežana Lj. Gojković[5], Vladislava M. Jovanović[1]
[1]ICTM - Department of Electrochemistry, University of Belgrade, Serbia, [2]IC Faculty of Technology and Metallurgy, University of Belgrade, Serbia, [3]Institute for Multidisciplinary Research, University of Belgrade, Serbia, [4]AGH University of Science and Technology, Krakow, Poland, [5]Faculty of Technology and Metallurgy, University of Belgrade, Serbia, [6]Serbian Academy of Sciences and Arts, Belgrade, Serbia

P.S.C.16. **Texture evolution of Cu single crystals after drawing**
Dorota Moszczyńska, Bogusława Adamczyk-Cieślak, Jarosław Mizera
Faculty of Materials Science and Engineering, Warsaw University of Technology, Woloska 141, 02-507 Warsaw, Poland

SYMPOSIUM D: ECO-MATERIALS AND ECO-TECHNOLOGIES

P.S.D.1. **Magnetite functionalized cellulose membranes for heavy metal removal from water**

Jelena D. Rusmirović[1], Jovana Nikolić[2], Dragana L. Milošević[2], Khaled Taleb[3], Milka Vidović[2], Aleksandar D. Marinković[4]
[1]Innovation Center of the Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11120 Belgrade, Serbia, [2]Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 4, 11000, Serbia, [3]Faculty of Engineering, Al-Jabal Al-Gharbi University, Gharyan, Libya, [4]Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11120 Belgrade, Serbia

P.S.D.2. **Application of NIR spectroscopy in study of adsorption process of p-nitrophenol on activated carbon in presence of selected amides**

Branko Kordić, Marina Kovačević, Tamara Sloboda, Branislav Jović
Department of Chemistry, Biochemistry and Environmental Protection, Faculty of Sciences, University of Novi Sad, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia

P.S.D.3. **Calorimetric research of arsenate adsorption on silica-based materials**

Vesna Rakić[1], Jelena Rusmirović[2], Aleksandar Marinković[2], Slavko Mijatov[2], Khaled Ahmed Taleb[3], Vincent Folliard[4], Georgeta Postole[4], Aline Auroux[4]
[1]Faculty of Agriculture, University of Belgrade, Nemanjina 6, 11080 Zemun, Serbia; [2]Faculty of Technology and Metalurgy,University of Belgrade, Karnegijeva 4, 11000 Belgrade, Serbia; [3]Faculty of Engineering, Al-Jabal Al-Gharbi University, Gharyan, Libya; [4]IRCELYON CNRS - Université Lyon 1, 2, Av. Einstein, 69626 Villeurbanne Cedex, France

SYMPOSIUM E: BIOMATERIALS

P.S.E.1. **Mono- and dinuclear azido Co(II) complexes with the condensation product of 2-quinolinecarboxaldehyde and Girard's T reagent**
Mima Romanović, Marko Jeremić, Milica Milenković, Božidar Čobeljić, Katarina Anđelković
Faculty of Chemistry, University of Belgrade, Studentski trg 12–16, 11000 Belgrade, Serbia

P.S.E.2. **Calvarial defects in rats filled with innovative nanocomposite material. Histological and biochemical studies**
Margarita Gabrashanska[1], Elena Dyulgerova[2], Radost Ilieva[2], Veselin Nanev[1], Ivelin Vladov[1], Petar Dimitrov[1], Neli Tsocheva-Gaytandzhieva[1]
[1]Institute of Experimental Morphology, Pathology and Anthropology with Museum, Bulgarian Academy of Sciences, Sofia, Bulgaria, [2]Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, Sofia, Bulgaria

P.S.E.3. **Biomimetic approach for preparation of calcium phosphate based cements**
Radost Ilieva[1], Rumiana Gergulova[1], Stefka Tepavitcharova[1], Kostadinka Sezanova[1], Anton A. Apostolov[2], Diana Rabadjieva[1]
[1]Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, Acad. G. Bontchev Str., Bl.11, 1113 Sofia, Bulgaria, [2]Faculty of Chemistry and Pharmacy, Laboratory of Polymers, Sofia University, 1, J. Bourchier Blvd., 1164 Sofia, Bulgaria

P.S.E.4. **Corrosion behavior of nanotubular oxide layer formed on titanium and Ti–13Nb–13Zr alloy processed by high pressure torsion**
Dragana R. Barjaktarević[1], Ivana D. Dimić[1], Ivana Lj. Cvijović-Alagić[2], Veljko R. Đokić[1], Jelena B. Bajat[1], Marko P. Rakin[1]
[1]Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4 11120 Belgrade, Serbia, [2]Institute of Nuclear Sciences "Vinča", University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia

P.S.E.5. **Effects of composition and method of preparation on biocompatible and biodegradable behavior of 3-D polymeric scaffolds based on gelatin/alginate/methacrylate**
Marija M. Babić[1], Jovana S. Vuković[1], Katarina M. Antić[1], Vuk V. Filipović[2], Simonida Lj. Tomić[1,*]
[1]Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, 11000 Belgrade, Serbia, [2]Institute for Chemistry, Technology and Metallurgy, University of Belgrade, 11000 Belgrade, Serbia

P.S.E.6. **Composite nanostructured HAp/YSZ dental inserts – processing, mechanical properties and application in dental restorations**
Giuma Ayoub[1], Đorđe Veljović[1], Maja Lezaja Zebić[2], Eriks Palcevskis[3], Vesna Miletić[2], Đorđe Janaćković[1]
[1]University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11120 Belgrade, Serbia, [2]University of Belgrade, School of Dental Medicine, DentalNet Research Group, Rankeova 4, Belgrade, Serbia, [3]Riga Technical University, Institute of Inorganic Chemistry, Miera 34, Salaspils, LV-2169, Riga, Latvia

P.S.E.7. **Novel composite alginate hydrogels with activated charcoal as a carrier of therapeutically active substances**
Andrea Osmokrović[1], Ivan Jančić[2], Jovana Vunduk[3], Nevena Dabović[1], Marina Milenković[2], Bojana Obradović[1]
[1]Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia, [2]Faculty of Pharmacy, University of Belgrade, Belgrade, Serbia, [3]Faculty of Agriculture, University of Belgrade, Belgrade, Serbia

P.S.E.8. **Towards a bio-nanoreactor by engineering inorganic nanoparticles with cancer cell membranes**
Vimal Balasubramanian[1], Alexandra Correia[1], Hong Zhang[2], Flavia Fontana[1], Ermei Mäkilä[3], Jarno Salonen[3], Jouni Hirvonen[1], and Hélder A. Santos[1,4]
[1]Division of Pharmaceutical Chemistry and Technology, University of Helsinki, Finland, [2]Department of Pharmaceutical Science, Åbo Akademi University, Finland, [3]Department of Physics and Astronomy, University of Turku, Finland, [4]Helsinki Institute of Life Science, HiLIFE, University of Helsinki, Finland

P.S.E.9. **Alumina based reinforcements for PMMA dental composite materials**
Gamal Lazouzi[1], Slađana Lakitić[1], Marija Dimitrijević[2], Nataša Tomić[2], Vesna Radojević[1], Radmila Jančić Heinemann[1]
[1]University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, Belgrade, Serbia
[2]University of Belgrade, Inovation Center of the Faculty of Technology and Metallurgy, Karnegijeva 4, Belgrade, Serbia

P.S.E.10. **Comparative spectroscopic characterization of fullerene nanomaterials**
Tamara Jovanović[1], Đuro Koruga[1], Branimir Jovančićević[2], Aleksandra Mitrović[3], Dragomir Stamenković[4], Ivan Rakonjac[3]
[1]Department of Biomedical Engineering, Faculty of Mechanical Engineering, University of Belgrade, Belgrade, Serbia, [2]Department of Applied Chemistry, Faculty of Chemistry, University of Belgrade, Belgrade, Serbia, [3]Innovation Center of Faculty of Mechanical Engineering, University of Belgrade, Belgrade, Serbia, [4]Optix, Inc., Belgrade-Zemun, Serbia

P.S.E.11. **3D finite elements modeling of the interfacial stresses bone/dental implant. Effects of the geometric parameters**

Toufik Outtas, Saida Ghoggali, Saber Latrèche
Laboratory of Mechanics of the Structures and Materials, University of Batna 2, Algeria

Abstracts

Oral Presentation

MRS-Serbia 2017 Award

Atomistic phenomena in engineering materials

Velimir R. Radmilović
Serbian Academy of Sciences and Arts, Knez Mihailova 35, 11000, Belgrade, Serbia, and
Nanotechnology and Functional Materials Center, Faculty of Technology and Metallurgy,
University of Belgrade, Karnegijeva 4, 11120 Belgrade, Serbia

As the recipient of this award I would like to thank the Materials Research Society of Serbia and my nominators, Professor Robert Sinclair of Stanford University and Dr. Ulrich Dahmen of the Lawrence Berkeley National Laboratory, as well as Dr. Dragan Uskoković, who coordinated the nomination and the decision making process, and many other colleagues who supported my nomination, for the honor of receiving this recognition. The results I will be presenting have been carried out not only by myself, but also by many of my graduate students and post-docs. Without their great talent and hard work none of these results would have been possible, and this recognition goes to them as well. I feel very honored to be given the opportunity to present an overview of the work from my group and the collaborations I've had throughout the years with some outstanding scientists from all over the world. Given the time constraint, I decided to present a few examples which demonstrate the main research interests of my group which are related to phase transformations in engineering systems, multi purpose thin film sensors and nanomaterials for energy related applications. The main research tools we have used were cutting edge characterization techniques, like aberration-corrected high resolution transmission electron microscopy in tandem with structure modeling and simulation, energy filtered spectrum imaging, electron energy loss spectroscopy, etc. The first example will demonstrate a way of producing coarsening resistant monodispersed $Al_3(LiSc)$ core/shell particles in an Al matrix, generated by a complex size focusing effect that drives the system in the opposite direction of typical Ostwald ripening. Our modeling and simulations show that the complex precipitation pathway can be fully understood within the framework of classical theories of nucleation and growth. The second example will show the potential of Al-Mo and Ni-Mo binary alloy thin films as resonating nanoelectromechanical system (NEMS) cantilever nanosensors, studied by means of microstructural and elastic properties measurements, using fiber optical interferometry. The third and final example will show our recent discovery of a novel method for synthesizing $M_2O_3(ZnO)n$ thermoelectric nanowires (MZO, M = In, Ga, Fe) using facile solid state diffusion, which enabled us to control their defect structure at an atomic level. Processing control at an atomic level will open up new avenues in synthesis of advanced materials with unprecedented mechanical and electronic properties.

I would like to acknowledge support from Serbian Academy of Sciences and Arts, under the project No. F-14.

PL.S.I.1.

Global opportunities in nanoscience and nanotechnology

Paul S. Weiss
California NanoSystems Institute and Departments of Chemistry & Biochemistry
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Two seemingly conflicting trends in nanoscience and nanotechnology are our increasing ability to reach the limits of atomically precise structures and our growing understanding of the importance of heterogeneity in the structure and function of molecules and nanoscale assemblies. By having developed the "eyes" to see, to record spectra, and to measure function at the nanoscale, we have been able to fabricate structures with precision as well as to understand the important and intrinsic heterogeneity of function found in these assemblies.

I will discuss the challenges, opportunities, and consequences of pursuing strategies to address both precision on the one hand and heterogeneity on the other. In our laboratories, we are taking the first steps to exploit precise assembly to optimize properties such as perfect electronic contacts in materials. We are also developing the means to make tens to hundreds of thousands of independent multimodal nanoscale measurements in order to understand the variations in structure and function that have previously been inaccessible in both synthetic and biological systems.

Another outcome of the development of our field has been our ability to communicate across fields. This skill that we develop in our students and colleagues has enhanced and accelerated the impact of nanoscience and nanotechnology on other fields, such as neuroscience and the microbiome. I will discuss the opportunities presented by these entanglements and give recent examples of advances enabled by nanoscience and nanotechnology.

PL.S.I.2.

Analysis of next generation Quantum Materials

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Depending on the composition, Quantum Materials may act as conductors, insulators, semiconductors or even as superconductors. Especially combinations of different quantum materials are of high interest to explore new phenomena and to build the foundation for future electronic devices at the nanometer scale. The properties of quantum materials differ strongly from the properties of their three dimensional bulk state. Our research on quantum materials is widely spread, reaching from defect formation in graphene to the characterization of hybrid quantum materials. We use low voltage aberration corrected electron microscopy to investigate chemical various quantum materials. In particular, we will present imaging and analysis of vapor deposition (CVD) graphene with added copper and mercury defects; graphene based hybrid structures, and FeSn Topological Insulators. We will also present our attempts of investigation of Vacancy centers in diamond. Further, correlation of the electron microscopy results with such techniques as EELS, Raman spectroscopy and Atom Probe, provides an excellent tool for understanding and correlating atomic structure and structural defects to the astonishing mechanical and electric properties of quantum materials. Advantages of utilizing low voltage aberration corrected electron microscopy for this type of materials will be presented as well.

PL.S.I.3.

Carbon nitrides as active semiconductors and supports for Artificial Photosynthesis and (Photo)Catalysis

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Polymeric graphitic Carbon Nitride can be made from urea under early-Earth conditions, as reported already by Justus Liebig in 1832. It just recently turned out to be a valuable extension to current semiconducting organic materials. This is due to the ease of synthesis, but also due to its extreme chemical stability. The resulting heterogeneous organocatalysts can- among other reactions- chemically activate CO_2 or photochemically split water into hydrogen and oxygen. This opens the door to artificial photosynthesis on the base of a sustainable and most abundant polymer base.

I will also present first schemes on generalizing the electronic properties of C_3N_4 to differently composed C/N-materials, successfully mimicking oxidation enzymes with high conversions and selectivity. The “hybridization” with enzymes via cofactor coupling allows synthesizing of more complex molecules photochemically, as shown by the chiral reduction of ketones by light. Another promising application is in electrodes for batteries and supercapacitors. Here C/N-technology is (foreseeable) able to replace rare metals for electron storage and electrocatalysis. I will exemplify some cases of materials with super-high surface area where new C/N-structures are used to design both the electrode structures as well as the redox shuffling and the catalytic conversions at the materials surfaces.

PL.S.I.4.

Efficient CRISPR delivery via plasmid DNA (or ribonucleoprotein, RNP) packaged in mesoporous silica nanoparticles through cationic vesicle fusion

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CRISPR systems are versatile tools for genome editing and transcriptional gene regulation. While the majority of delivery vehicles for genome editing, including CRISPR, have been viral, there are limitations to these vectors including carcinogenicity and immunogenicity. Non-viral vectors have a lower immunogenicity profile than viral vectors, however, so far, non-viral vectors have demonstrated limited delivery efficiency, due to the size and complexity of the cargo (plasmid DNA or the Cas9 endonuclease/gRNA ribonucleoprotein complex (RNP)) and the need to deliver it to the nucleus of the target cell. To address the CRISPR delivery problem, we developed a CRISPR plasmid delivery system based on mesoporous silica nanoparticles (MSN) encapsulated within supported lipid bilayers (aka protocells). MSNs have tailorable pore size (2-20-nm) and intrinsically negative surface charge. Although the pore size is not large enough to accommodate plasmid DNA, we discovered that we can package negatively charged plasmids via fusion of cationic lipid vesicles on MSNs and that the MSN pore size is a major determinant of plasmid loading efficiency. Using dynamic light scattering, cryo-TEM, and high resolution confocal imaging, we have proven the plasmid-packaged protocells to be stable monosized colloids wherein DNA is co-localized with MSNs and protected within a supported lipid bilayer or multilayer. Protocells exhibit high levels of DNA loading and protection of DNA from nuclease degradation while maintaining a ~200nm hydrodynamic diameter and low polydispersity suitable for in vivo delivery. In vitro gene editing efficiencies were greater than 80%, equal to those seen with high dose lipofectamine, but with far lower toxicity. We hypothesize that the high gene editing efficiency is a consequence of spontaneous disassociation of the negatively charged DNA from the negatively charged MSN when the supported lipid bilayer is destabilized within the acidic endosomal environment following protocell internalization. To demonstrate CRISPR gene editing in a living system, we utilized the vascularized chick chorioallantoic membrane (CAM) model and intra vital imaging. Protocells successfully delivered CRISPR encoding plasmids to human A549 cells through the CAM vasculature resulting in expression of CRISPR Cas9 and editing of a reporter gene system after 24 hours. Further, we demonstrated the same cationic vesicle packaging approach could also be used for RNP delivery.

PL.S.I.5.

“Anything You Can Do I Can Do Better”
What can be done with Sonochemistry?

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Sonochemistry is the research area in which molecules undergo chemical reaction due to the application of powerful ultrasound radiation (20 KHz - 1 MHz). The physical phenomenon responsible for the sonochemical process is acoustic cavitation. A number of theories have been developed in order to explain how 20k Hz sonic waves can break chemical bonds. They all agree that the main event in sonochemistry is the creation, growth, and collapse of a bubble that is formed in the liquid. The stage leading to the growth of the bubble, occurs through the diffusion of solute vapor into the volume of the bubble. The last stage is the collapse of the bubble, which occurs when the bubble size reaches its maximum value. We will adopt the hot spot mechanism, one of the theories that explain why, upon the collapse of a bubble, chemical bonds are broken. The theory claims that very high temperatures (5,000-25,000 K) are obtained upon the collapse of the bubble. Since this collapse occurs in less than a nanosecond, very high cooling rates, in excess of 10^{11} K/sec, are also obtained. This high cooling rate hinders the organization and crystallization of the products. The results of the many reactions carried out by my group and by others show that the products were having always nanometric size, but so are 40-50 other methods by which nanomaterials are prepared. The question is therefore asked what are the advantages of using sonochemistry. I will mention and discuss four such advantages. 1) Preparation of amorphous products. 2) Insertion of nanomaterials into mesoporous materials. Ultrasonic waves are used for the insertion of amorphous nanosized catalysts into the mesopores. A detailed study demonstrates that the nanoparticles are deposited as a smooth layer on the inner mesopores walls, without blocking them. When compared to the other methods such as impregnation or thermal spreading sonochemistry shows better properties. 3) Deposition of nanoparticles on flat and curved surfaces. We have immobilized a large variety of nanomaterials on metals, ceramics, polymers, glass, textiles, and paper, imparting a large variety of properties such as magnetic, conductive, antibacterial, antiviral, antibiofilm and more to the substrates. The adherence of the |nanomaterials to the substrate was demonstrated when cotton coated by CuO nanoparticles were washed 65 cycles in Hospital washing machines (92 deg. cent.) and the fabric was found highly antibacterial after this long washing. 4) The formation of micro and nanospheres of proteins, DNA, RNA, starch, chitosan and more. The encapsulation of drugs in the spheres will be demonstrated. The use of the DNA nanospheres for gene silencing will be discussed.

PL.S.II.1.

Assessing material reactions in the environmental transmission electron microscope (TEM)

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The environmental transmission electron microscope (ETEM) allows the study of material reactions in situ, in a mild gaseous environment, at atomic resolution. Higher pressures and liquids are possible with a closed-cell specimen holder, albeit at lower resolutions [1]. Such studies represent the fastest growing field within in situ TEM. In this paper, we will assess the results obtained in situ compared with equivalent ex situ or low electron beam dose rate observations. It will be seen that on occasion the imaging electron beam can mimic important real experimental conditions while many times it induces completely different results. Specific systems to be considered include the hydrogenation of amorphous molybdenum sulphide [2], the reduction of epitaxial ceria thin films [3] and the oxidation of carbon nanotubes [4]. The care necessary to ensure reliable observations will then be emphasized.

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PL.S.II.2.

In-situ microscopy with atomic resolution at atmospheric pressure

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Understanding the atomic structures of catalysts under realistic conditions with atomic precision is crucial to design better materials for challenging transformations. For example, under reducing conditions, certain reducible supports migrate onto supported metallic particles and create strong metal−support states that drastically change the reactivity of the systems. The details of this process are still unclear and preclude its thorough exploitation. In the past decade, most of atomic-scale transmission electron microscopy (TEM) studies involving gas-solid interactions were conducted in an environmental TEM, where the gas pressure is typically limited to less than 1/100 of atmosphere. Recently, it has become possible to overcome this limitation through a MEMS-based, electron-transparent closed cell with a heating stage.

In this talk, I will present our recent results using this device (the Protochips AtmosphereTM system) in selected catalyst systems. In a palladium/titania (Pd/ TiO_2) catalyst, we directly observed the formation of the oxide overlayers on the supported Pd particles with atomic resolution under atmospheric pressure and high temperature. It shows that an amorphous reduced titania layer is formed at low temperatures, and that crystallization of the layer into either mono- or bilayer structures is dictated by the reaction environment. This transition occurs in combination with a dramatic reshaping of the metallic surface facets. In-situ TEM observations of a modular Pd-ceria core-shell nanostructured catalyst ($Pd@CeO_2$) showed that an unexpected structural transformation occurs upon heating at high temperatures. The system reaches to a stable state with the mixture of nanoparticles with two different sizes, which accounts for the exceptional catalytic properties that have been reported. Using the similar techniques, we also studied the core-shell platinum-metal (Pt-M) nanoparticles which show a catalytic performance in the oxygen reduction reaction (ORR) superior to that of pure Pt nanoparticles. To understand the formation mechanism of the Pt shell, we studied thermally activated core-shell formation in Pt_3Co nanoparticles via in-situ electron microscopy with the gas cell. The disordered Pt_3Co nanoparticle was found to transform into an ordered intermetallic structure after annealing at high temperature (725 °C) in 760 Torr O_2, followed by layer-by-layer Pt shell growth on (100) surfaces at low temperature (300 °C). The apparent 'anti-oxidation' phenomenon promoted by the ordered Pt_3Co phase is favorable to the ORR catalyst, which operates in an oxidizing environment.

PL.S.II.3.

In situ advanced electron microscopy of nanostructured materials for energy and quantum devices

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In situ electron microscopy reveals the correlation between local material structure and properties and also allows the correlation to be studied on different length scales spanning from the subatomic dimension to micrometers. We can study electrically, mechanically and thermally induced changes of charge transport properties using holders designed to enable different stimuli. 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 different length scales. This talk addresses examples of in situ electrical and thermal studies combined with advanced imaging and spectroscopy techniques [1-3].

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PL.S.II.4.

Atomic resolution imaging of materials in the chromatic and spherical aberration corrected transmission electron microscope

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In a chromatic and spherical aberration corrected electron microscope the two major resolution limitations of previous generations of instruments due to partial spatial and partial temporal coherence are significantly reduced. As only recently discovered the spatial resolution of such an instrument is limited by a previously concealed residual image spread whose origin is thermal nanomagnetic field-noise, also known as Johnson noise. The Juelich Titan 60-300 PICO instrument is the first (recently) equipped with an aberration corrector minimizing the effect of Johnson noise. We report on resolution tests demonstrating a record resolution for TEM of 48 pm at 200 keV, and we demonstrate a practical materials science resolution of 57 pm in an investigation of $YAlO_3$:Ce. Another unique advantage of spherical and chromatic aberration correction is energy-filtered TEM for which we demonstrate by imaging of the Si [110] dumb-bell atom pairs with electrons having suffered a L2,3 core loss a record resolution of 1.35 Å at 300 keV.

PL.S.II.5.

Model-based reconstruction of magnetisation distributions in nanostructures from electron-optical phase images

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The development of an experimental technique that allows the three-dimensional magnetic state of a nanoscale object to be measured quantitatively is of great importance for fundamental and applied research in nanomagnetism. Off-axis electron holography is a powerful technique that can be used to record the phase shift of an electron wave that has passed through a specimen in the transmission electron microscope (TEM). The phase shift is, in turn sensitive to the in-plane component of the magnetic induction within and around the specimen projected in the electron beam direction.

We are currently developing a model-based approach to magnetic vector field tomography, which involves using an iterative reconstruction algorithm to recover the three-dimensional magnetization distribution in a specimen from a series of magnetic phase images recorded using electron holography as a function of sample tilt angle. The advantage of using such a model-based approach is that each trial solution is guaranteed to satisfy known physical laws. In order to optimise the speed of the algorithm, pre-computed analytical solutions for the phase contributions of simple geometries are used to avoid full matrix calculations. Together with an efficient use of Fourier space convolution, this approach significantly speeds up the reconstruction process, while minimising memory consumption.

The initially ill-posed problem is first replaced by a least-squares minimisation problem. First order Tikhonov regularisation is applied, motivated by minimisation of the exchange energy of the magnetisation distribution. A mask is introduced to localise magnetised objects and to decrease the number of unknowns. All measures are combined into a cost function, whose minimisation, facilitated by conjugate gradient methods, replaces the original problem. Diagnostic tools are used to assess the quality of the reconstruction result. The regularisation strength and the choice of mask are found to significantly influence the resolution of the reconstruction. Sources of magnetisation outside the field of view are accounted for by introducing buffer pixels. Perturbation of the hologram reference wave, which originates from long-reaching stray fields from the magnetised object, are addressed by modifying the convolution kernels. A confidence array is used to exclude other identifiable artefacts from the reconstruction process. Examples of the application of the algorithm to the recovery of selected three-dimensional magnetization distributions will be presented [1].

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PL.S.II.6.

Atomic resolution TEM characterization of GaSb/GaInAs and GaSb/GaInP bond interfaces for high-efficiency solar cells

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Multi-junction solar cells based on III-V semiconductors reach the highest conversion efficiencies and are currently used primarily in concentrator photovoltaic systems and for power generation on satellites or spacecraft. Several cells of different III-V compound semiconductor materials are generally combined to absorb a different wavelength range of the solar spectrum and to convert it into electric power. Fabrication of these cells by wafer bonding is of interest since efficiencies of up to 46 % have been obtained [1], and efficiencies of up to 50% are within reach. Fast atom beam activation is generally used as a pre-treatment to remove oxides and contamination before bonding [2]. Activation treatment and bond processing often result in the formation of amorphous interface layers with inadvertent impurities [3]. We have applied high-resolution imaging and spectroscopic techniques of transmission electron microscopy (TEM) techniques to investigate the interface regions of in as-bonded and thermally annealed (at temperatures of $T \leq 500$ºC) GaSb/GaInAs and GaSb/GaInP layer systems. We, combining used aberration-corrected high-resolution TEM, high-angle annular dark-field scanning (S)TEM, and energy-dispersive X-ray spectroscopy (XEDS) using with an aberration-corrected probe that allows to monitor elemental distributions with high precision and with sub-nanometer spatial resolution.

For GaSb/GaInAs, we find that the crystal lattices are interconnected. The bond interfaces reveal exhibit terraces, misfit dislocations, and nanometer-sized pores, as well as element compositional fluctuations in the near-interface regions. For GaSb/GaInP, the interface regions are characterized by an amorphous interlayer that has a thickness of approximately about 1.5 nm, thick and reveal with a minor enrichments of Ga. These phenomena are attributed to the wafer pre-treatment before bonding. Thermal annealing, which is - often employed used as a method to for improving the interface conductance, - results in changes of their structure and element composition. The amorphous interlayers are reduced their in thickness by recrystallization, resulting in a largely epitaxial interface at after annealing at 500 ºC. XEDS mappings reveals detectable amounts of In and P for after annealing at temperatures $T \geq 225$°C, as well as small pores and In-rich crystalline precipitates for $T \geq 400$°C) in the GaSb near-interface regions. These observations allow to provide an understanding of the electrical properties of these interfaces [4] and are discussed also in view of can be compared with results obtained for from GaAs/Si wafer-bond interfaces [3]. From a methodological point of view, these examples our results show how the applied methods of aberration-corrected TEM can be used to contribute to the monitoring, control, and optimization of concepts for the fabrication of high-efficiency solar cells. An optimized 4-junction solar cell based on GaInP/AlGaAs//GaInAs/Ge currently has an efficiency of 38.5 % under a concentration of 188 suns, while and a GaInP/GaAs/GaInAs//GaSb cell has a first efficiency of 29.1 % under 194 suns [1].

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PL.S.II.7.

Sub-30 meV energy resolution HR-EELS and novel HR-STEM techniques for materials science in the latest generation of Thermo Scientific Themis Z

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In order to address increasing interest of materials science community towards higher spatial resolutions, lower working high tensions and innovative STEM imaging methods, Thermo Scientific has recently released its latest Themis Z generation. It will be capable of answering most of present and future needs in terms of producing fast, sensitive and unrivaled quality data from challenging samples.

With unprecedented TEM and STEM spatial resolutions from 300 kV down to 30 kV, Themis Z provides the best resolving power for any materials science specimen. New OptiSTEM+ software automatically corrects for STEM defocus and aberrations (up to all second order) in a single click, making it possible to get the best out of the microscope at each image. Another user-friendly package, OptiMono, automatically excites the monochromator for HREELS studies (plasmonics, band gap determination, ELNES) as well as for low kV TEM and STEM studies. With new iDPC STEM imaging technique (integrated Differential Phase Contrast), low- and high-Z atoms are simultaneously imaged at very high S/N ratio, single defocus value, and without any contrast reversal. Moreover, iDPC, due to high S/N ratio, is an ideal imaging method for low dose STEM studies on beam sensitive specimens (2D materials, zeolites, polymers, cryo-sections, ...).

With Thermo Scientific NanoEx in-situ holders, Themis Z itself becomes a well-equipped nano-laboratory. Furthermore, Ceta camera with speed upgrade providing high-resolution (4k x 4k) and high-definition movies at a speed of more than 30 fps is able to successfully record all sample transformations during dynamic experiments without risking to miss any information. Extra focus during the speech will be put on pixelated detectors, 4D STEM applications, and UHR EELS capabilities. In particular the EELS spectroscopy will see a revolution capitalizing on better than 15 meV energy resolution on a millisecond base and at 60 kV. Such a great performance is available for the very first time in a versatile STEM/TEM Transmission Electron Microscope like Themis Z.

PL.S.III.1.

Nanoparticles as delivery vehicles: Enabling nanocomposites and healthcare

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The past thirty years has seen an ever-increasing interest in nanoparticles of a variety of elemental constituents, sizes and morphologies, which have been used as the building blocks of nanostructured materials and devices with unique properties and functionalities. These materials and devices have enabled the continued development of nanotechnology for the increasing benefit of society. The special properties of nanoparticles, with their inherent nanoscale topography, their very large surface-to-volume ratios, along with our ability to precisely functionalize their surfaces, have created through recent experiments a novel view of them as powerful delivery vehicles with great potential for enabling novel multifunctional nanocomposite materials and multiple healthcare applications. A brief commentary on this exciting and ever-developing field, with examples highlighted from our research efforts at Rensselaer, will be presented that focuses on a number of current advances in our understanding that indicate some opportunities for solutions to important societal problems.

PL.S.III.2.

Multifunctional nanocarriers for drug delivery in cancer therapy

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Tumor therapy, especially in the case of multidrug resistant cancers, could be significantly enhanced by using siRNA down-regulating the production of proteins, which are involved in cancer cell resistance, such as Pgp or survivin. Even better response could be achieved is such siRNA could be delivered to tumors together with chemotherapeutic agent. This task is complicated by low stability of siRNA in biological surrounding. Thus, the delivery system should simultaneously protect siRNA from degradation. We have developed several types of lipid-core polymeric micelles based on PEG-phospholipid or PEI-phospholipid conjugates, which are biologically inert, demonstrate prolonged circulation in the blood and can firmly bind non-modified or reversibly-modified siRNA. Additionally, these nanopreparations can be loaded into their lipidic core with poorly water soluble chemotherapeutic agents, such as paclitaxel or camptothecin. In experiments with cancer cell monolayers, cancer cell 3D spheroids, and in animals with implanted tumors, it was shown that such co-loaded preparations can significantly down-regulate target proteins in cancer cells, enhance drug activity, and reverse multidrug resistance. In order to specifically unload such nanopreparations inside tumors, we made them sensitive to local tumor-specific stimuli, such as lowered pH, hypoxia, or overexpressed certain enzymes, such as matrix metalloproteases. Using pH-, hypoxia-, or MMP2-sensitive bonds between different components of nanopreparations co-loaded with siRNA and drugs, we were able to make the systems specifically delivering biologically active agents in tumors, which resulted in significantly improved therapeutic response.

PL.S.III.3.

Targeted nanomedicines for cancer, diabetes and cardiovascular diseases: why the size matters?

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Explosive growth of nanomedicines continues to significantly impact the therapeutic strategies for effective cancer treatment. Despite the significant progress in the development of advanced nanomedicines, successful clinical translation remains challenging. However, novel biomedical engineering technologies have been underlined as very promising means for the advance in medical research [1–3]. Personalized medicine allows for the identification of the right therapy, reaching the right therapeutic target in the body at the right time in an efficient manner, with reduced undesired collateral effects [4]. In this context, target nanomedicines are of great interest towards the development of personalized medicines and envisaged for their large-scale implementation. Recently, we have developed prominent biomaterials, such as porous silicon and polymer-based micro/nano-particles as potential platforms for cancer theranostics and other individualization of medical intervention [5–13]. All these biomaterials are promising advanced drug delivery technologies for biomedical applications. The results of the efficient surface biofunctionalization, targeting, imaging, encapsulation of drug molecules using advanced technologies, such the microfluidics technique, are presented and discussed in detail. Examples on how these materials can be used to enhance the bioavailability of drug/peptide molecules, demonstrating their cytocompatibility, in vivo biofate (imaging) and intracellular cancer targeting, are also discussed for different biomedical applications. Overall, the recent cutting-edge advances on nanomaterials are anticipated to overcome some of the therapeutic window and clinical applicability of many drug/peptide molecules and, thereby, hopefully enhancing the expectancy and quality of life of the patients.

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PL.S.III.4.

Bioinspired biomaterials for hard tissue repair and regeneration

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Bone and dentin are mineralized hard tissues. The primary inorganic component is crystalline hydroxyapatite and type I collagen forms the template for mineral deposition. Tissue engineering strategies using novel biomaterials have emerged as a promising potential for treatment of mineralization defects. A key functional property is that biomaterials need to be cell-compatible and mimic the dynamic nature of the extracellular matrix. Novel biomaterials that are currently being developed are protein-engineered biomaterials that would mimic the ECM environment of cells. Recently, peptide-based engineered hydrogel scaffolds have been developed and they present several advantages over traditional protein scaffolds. The control over hydrogel properties can be easily manipulated and tailored to the requirement of the tissue. Biomaterials generated by the self-assembly process have varied applications as it mimics nature's method of material synthesis. Therefore, concepts of synthesizing biomaterials can be adapted from nature for constructing useful biomaterials for hard tissue regeneration.

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PL.S.III.5.

Design of materials properties by microstructure and external fields

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The mechanical, physical and chemical properties of materials are determined by their microstructure. Modern materials science uses the complex interplay of defects, such as impurities, phases, point and line defects and interfaces, to tailor properties and obtain high-performance metallic alloys and ceramics. In this approach of materials design, properties can only be changed by modifying their microstructure, for example by initiating grain growth during annealing at elevated temperatures. Such a behavior, that fixes the properties irreversibly to the microstructure, is advantageous for many applications of materials, where long-term stability of the properties is required.

Two examples for designing materials properties will be presented, nanoglasses and equiatomic multicomponent single phase oxides.

Metallic glasses offer interesting properties due to their disordered atomic structure. Due to the fact that they are prepared predominantly by rapid quenching, only a certain range of microstructural parameters has yet been explored. As an example for materials that exhibit novel effects by tailoring the microstructure, nanoglasses will be discussed. Nanoglasses consist of two distinct structural components, which differ in their free volume and elemental constitution, and have been shown to exhibit drastic property changes.

Equiatomic multicomponent single phase oxides, oxides with simple crystallographic structures consisting of up to 10 different cations, have been prepared by different synthesis routes. Nebulized spray pyrolysis has been shown to be the most flexible and versatile technique. Some examples of different structures for transition and rare earth metal oxides and perowskites will be presented.

In contrast, tuning using external fields, i.e., electric, offers completely new opportunities for the fully reversible control of materials properties. Such tuning of physical properties will be demonstrated for several nanostructures, i.e. (epitaxial) thin films, nanoporous, nanoparticulate structures and nanowires. Tuning can be either achieved using dielectric/ferroelectric gating, well known from semiconductor physics, or by electrolyte gating using liquid or solid electrolytes. Furthermore, using electrochemical ion intercalation, fully reversible properties with substantially larger effect magnitude can be achieved.

Finally, the concepts employed for tuning properties of nanostructures can be employed in applications as well. As an example, field-effect transistors based on inorganic nanoparticles as the channel material and solid electrolyte for the gating will be described.

PL.S.III.6.

Sucking the heat out of ceramic processing

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For over 30,000 years, the general practice of sintering ceramics has involved a high temperature thermal treatment to drive the transport processes to densify the particles and minimize the surface energy of the material. Typical sintering temperatures consider 0.6 to 0.8 of the melting temperature (Tm) for many oxides; this means we sinter around 800 ºC to 1200 ºC for 2 to 10 hours. Here we introduce a broad body of systems that utilize a transient aqueous based liquid phase (1 to 10 wt%) that sinters under a uniaxial pressure, while being heated from room temperature to 250 ºC, over a time period of 10 to 60 minutes. During this process, there are all the aspects of liquid phase sintering, namely particle rearrangement, dissolution precipitation, and grain growth. We believe transport processes are enhanced through mechanisms such as diffusiophoresis, which in turn is driven by concentration gradients. This phenomenon has very fast transport velocities, and therefore does not require high temperatures ~ 10 micrometers/sec. The driving for precipitation is also enabled by the transient evaporation of the water and a sustained supersaturation under local hydrothermal conditions. These mechanisms work together to create a pathway to sinter ceramics under extremely low temperatures and fast times; many of the systems that we will show are sintered at 120 ºC, 15 minutes, under 300 MPa uniaxial pressure. We have termed this fabrication method the Cold Sintering Process (CSP). We fully realize that there are many subtle differences in the CSP of each system, but as this is the start of a new approach, we will share our qualitative understanding, as determined from microstructural observations. We have also benchmarked and compared properties where possible, and it will be seen that the properties are in comparison to conventionally processed materials; we will in particular contrast conduction and dielectric properties.

Given the massive drop in sintering temperature of the ceramic, this offers many new opportunities in material design, especially in composites. We will show three different types of polymer ceramic composites with high percentages of ceramic, 100% to 60%, with the thermoplastic polymers for dielectric applications, ionic electrolytes, and semiconducting composites. We will also show preliminary data with CSP with multilayer ceramics and printable electronics.

PL.S.III.7.

Materials characterization and integrated computational materials engineering: Providing solutions for near-net shape manufacturing

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There have been, over the past four decades, various processing schemes introduced that are focused on near net-shape manufacturing of components. These are often based on powder metallurgy approaches, and include hot isostatic pressing (HIP) and additive manufacturing (AM). The full exploitation of these processing schemes has been frustrated by a number of limiting factors including anisotropic and coarse microstructures, issues with prior-particle boundaries, porosity, residual stress, and deficits in certain mechanical properties. This presentation describes an effort aimed at overcoming some of these problems through application of a combination of sophisticated materials characterization and integrated computational materials engineering. The focus has been on the production of equiaxed microstructures and improved fatigue properties of Ti alloys, and the reduction of the influence of ppb's in Ni-base superalloys. The results of these experiments will be discussed in terms of the increased use of these processing approaches for the manufacture of turbo-machinery.

PL.S.IV.1.

From low dose In-line electron holography to atomic resolution tomography

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To address Feynman's dream, it is important to extract 3D atomic coordinates in a nano-object [1]. So far, there are two approaches, namely, STEM-tilt series [2] and in-line holography [3] have been demonstrated to achieve the atomic resolution tomography for fulfilling Feynman's dream to understand physical and chemical properties of nano-object. Most noticeable bottleneck is the large accumulated electron dose required to produce tilt series of atomic resolution images, because electron dose are commonly chosen large (10^4 -10^5 e$Å^2$ s -1) to achieve a needed resolution around 1Å and single atom sensitivity. Any such single image can exhibit uncontrolled electron beam-induced surfaces alterations or even bulk modifications, in particular if particles are small or for the organic materials such as protein or molecules. For biological sample, protein, the 3D structure is usually reconstructed from images recorded at the cryo-mode to slow down the electron radiation damage. But drawback of cryo-microscopy is that at the low temperature the shape of the protein will be deformed. And the proteins are required exists high symmetry for cryo-microscopy with single particle reconstruction. In my talk, we present a self-consistent approach to recover the 3D atomic structure of nanocrystalline particles from single projections by exploiting the dynamic nature of electron scattering and pursuing a quantitative interpretation of the electron exit wave reconstructed from focal series of high-resolution images recorded at low dose mode. Beyond investigations of radiation hard periodic matter, the approach offers intrinsic advantages to study beam-sensitive materials such as catalysts and molecules because dose-rate dependences can be exploited to help reducing beam-sample interactions so that atomic resolution and single atom sensitivity may be achieved without altering the pristine structure of radiation sensitive matter. In my talk, we demonstrate the 3D information of the atomic position in encoded in the exit wave function reconstructed from simulated focus series images. The positions of exit surface atom, and therefore the surface profile, can be determined from the maximum intensity of the propagation wave with an accuracy of atomic resolution [3]. The number of atom in a column can be quantitatively counted from the relative phase angle of the focus corrected wave and the vacuum wave [3]. Several cases of the reconstructed atomic resolution tomograms, such as Au nano-bridge, Ge wedge crystal, and MgO nano-cube will be demonstrated.

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PL.S.IV.2.

Electron holography of nanoscale electric and magnetic fields

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Off-axis electron holography in the transmission electron microscope provides a unique and powerful approach to visualizing electric and magnetic fields within materials with resolutions approaching the nanometer scale. The ability to image phase shifts at medium resolution opens up a wide field of interesting and important materials problems. In this work, the technique has been successfully used to quantify electrostatic and magnetic fields in and around deep-submicron devices and patterned nanomagnets. An important extension of this work has involved in situ application of magnetic fields to image local magnetic response during hysteresis loops. Applications include asymmetric pinning of domain walls at notches in nanowires. Electrostatic field examples include, imaging of electrostatic phase shift at quantum dots to allow for quantification of charge capture and measurement of piezoelectric fields and 2-dimensional electron gas densities. In situ biassing of doped Ge-Si nanowires allows for analysis of activation of dopants.

PL.S.IV.3.

Complex heterostructures investigated using aberration-corrected STEM

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This talk will review some of our recent studies of heterovalent semiconductor interfaces and oxide/oxide or oxide/semiconductor heterostructures. The systems studied include several pairs of Group II-VI/Group III-V compound semiconductors with zincblende structure, and various oxides grown either on strontium titanate (STO) or on Si(001) and Ge(001) substrates. In the former pairs of semiconductor materials, lattice mismatch plays a major role in controlling the types of interfacial defects observed. For the oxides grown on STO, changes in the titanium oxidation state close to the interface result in the creation of a two-dimensional electron gas. For the oxide/semiconductor combinations, minimization of mismatch strain can be used as a strategy to control crystallographic orientation and hence the polarization direction.

Acknowledgments: Ongoing collaborations with the groups of Alex Demkov and John Ekerdt (University of Texas-Austin) and Yong-Hang Zhang (Arizona State University) are gratefully acknowledged.

PL.S.IV.4.

Pushing the limits of electron energy loss spectroscopy for materials characterization: from phonons to core losses in real and momentum spaces

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A new generation of monochromators has recently pushed the energy resolution of (scanning) transmission electron microscopes into the sub 20meV range. In addition to the obvious increase in resolution which has made exploring the phonon region of the electron energy loss spectrum (EELS) possible, the flexibility of these instruments is proving advantageous for materials science investigations. The energy resolution, beam current and optics can be adjusted seamlessly within a greatly increased range. This contribution will illustrate these possibilities through a number of systems, such as a highly promising A-site deficient $Nd_{2/3}TiO_3$ based perovskite system. Using monochromated core loss EELS it is for instance possible to map individual components of the Ti L2,3 edge at atomic resolution and relate them to structural distortions of great importance for the material’s properties.

PL.S.IV.5.

Corrosion at the Nanoscale: the role of chloride

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Corrosion is a pervasive phenomenon, which despite decades of study is still not well understood at the nanoscale. While water is itself corrosive, when chloride ions are present many protective oxide films break down. Understanding this is critical for both applications in salt water and in-vivo, since both have high levels of chloride. After a general introduction, this talk will focus on the effect of chloride. I will show using density functional calculations that the dominant effect is an anisotropic change in the surface energy. The theoretical analysis is then combined with experimental TEM and APT studies which corroborate with the theoretical results.

PL.S.IV.6.

Sub-100nm in-situ X-ray tomography – Applications in materials science and engineering

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High-resolution nondestructive studies of kinetic processes in materials is a highly ranked request from advanced materials development, and it is an industrial demand for reliability engineering in several branches including microelectronics, energy storage and lightweight construction. There is a particular need for 3D structural and chemical characterization of materials and devices with a spatial resolution of 100 nm and below. Due to the particular properties of X-rays, i. e. high penetration of matter and good material contrast in absorption, nano X-ray tomography is a versatile tool for nondestructive 3D bulk analysis of materials and for the investigation of complex 3D structures. Examples for high-resolution in-situ X-ray imaging studies will be shown, including studies of kinetic processes in materials: Physical failure analysis in 3D-stacked microchips, kinetic reactions for energy storage and conversion processes, crack initiation and propagation in microchips and composites.

Novel focusing lenses, so-called multilayer Laue lenses, have the potential to bring hard X-ray microscopy (high photon energy) at high efficiencies to resolutions down to the 10 nm range and below, since the resolution is not limited by the patterning process as applied for the fabrication of state-of-the-art Fresnel zone plates. Full-field imaging, demonstrated first time in a laboratory X-ray microscope using multilayer Laue lenses, will be reported. Combined with a larger focal length, nano X-ray tomography of larger samples is possible, and space is available to insert in-situ experimental setups (micromechanical testing, reaction chambers, high temperature/cryo stages) in the beam path.

PL.S.IV.7.

Atomic level characterization of novel hardening mechanisms in high-Mn-steels

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Recently developed high-manganese steels exhibit an exceptional combination of strength and ductility and show great promise for structural applications. Understanding the relationships between manganese and carbon content, microstructure, temperature, defect formation and strain-hardening behavior is critical for further optimization of these steels. We investigated the influence of alloy content, temperature and deformation behavior on the microstructural evolution of an austenitic Fe-14Cr-16Mn-0.3C-0.3N alloy showing twinning induced plasticity (TWIP) and of a two-phase nanostructured Fe-30.5Mn-8Al-1.2C alloy exhibiting microband induced plasticity (MBIP). The twinning induced plasticity (TWIP) effect enables designing austenitic Fe-Mn-C based steels with >70% elongation at an ultimate tensile strength >1 GPa. High resolution TEM and STEM images of the planar defects will be presented and detailed investigations revealed insight in the atomistic structure of defects and defect/dislocation interaction. In the MBIP alloys, regularly spaced coherent precipitates of the κ-Phase were found, which cause the unique properties of these materials.

PL.S.IV.8.

Solid-solid interface reconstruction at nominally incoherent interfaces: Ni-Al_2O_3 and Ni-YSZ

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Atomistic characterization of interfaces usually focuses on low-index orientations where semi-coherent interfaces can be described using misfit dislocations separating regions of coherency. However, many systems are incoherent due to significant differences in lattice symmetry and/or lattice parameters. Mechanisms for strain compensation at incoherent interfaces have been largely ignored.

In this presentation the structure of equilibrated Ni-sapphire and Ni-YSZ interfaces will be presented. Equilibrated Ni particles were formed by solid-state dewetting of Ni films on the substrates. Aberration corrected scanning transmission electron microscopy (S/TEM) showed that the Ni-sapphire(0001) interface is incoherent, and reconstructs to form a 2.5√3R30 2-D lattice. The more than 30% mismatch between Ni and YSZ leads to a nominally incoherent interface, containing a high density of semi-periodic misfit dislocations which define the reconstructed interface. The concept of interfacial reconstruction as mechanism for compensating strain energy will be discussed.

O.S.F.1.

Platinum monolayer fuel cell electrocatalysts

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Fuel cells, the devices that convert directly chemical energy of fuels into electrical energy, are considered to become a major source of clean energy. Particularly attractive is their automotive application that would produce enormous environmental benefits. A widespread application of fuel cells has been hampered by i) the cost of the catalysts (Pt) for fuel oxidation and oxygen reduction reactions, ii) their insufficient activity and iii) inadequate stability.

Although considerable advances in developing fuel cell catalysts were made over the last fifteen years, the amount of platinum used in electrocatalysts for the oxygen-reduction reaction (ORR) at fuel-cell cathodes remains large because of its insufficient catalytic activity and stability. In addressing those drawbacks, we developed Pt monolayer (Pt_{ML}) electrocatalysts consisting of a single-layered shell of Pt atoms on cores of metal- or alloy- nanoparticles[1],[2]. The origin of their high activity was identified by electrochemical- and surface-science techniques, x-ray absorption spectroscopy, and density functional theory calculations. The Pt monolayer electrocatalysts offer several uniquely attractive properties including an ultra-low Pt content, 100% Pt utilization and very high activity. High stability induced by supporting nanoparticle cores, self-healing property and fuel cell tests indicate that these electrocatalysts are ready for application and are established as a viable practical concept[2,3,]. Further improving of these electrocatalysts can be achieved by changing the composition, shape, and size of cores to optimize the core-shell interaction, thus tuning their activities (Figure 1). The unique features of Pt_{ML} electrocatalysts enable a wide selection of substrates to attain an electrocatalyst having low noble-metal content with enhanced catalytic activity and stability.

Several synthetic processes can be used to obtain the supporting cores, while the main method for placing a Pt monolayer on these core-shell nanoparticles involved the galvanic displacement of a Cu monolayer obtained by underpotential deposition by Pt. Other properties and further improvements of these catalysts will be discussed at the meeting.

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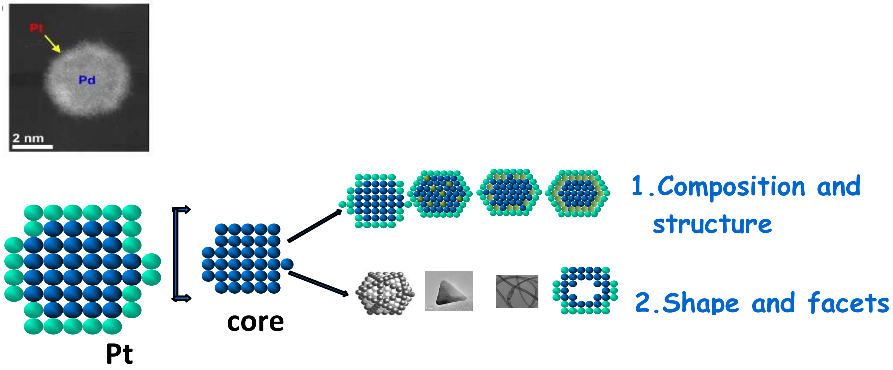

Figure 1 SEM image of a Pt monolayer shell on a Pd core nanoparticle (left panel). Schematics of possible ways for tuneing Pt monolayer catalysts properties through core-shell interactions.

O.S.F.2.

Energy and fuels from electrochemical interfaces

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Developing and deploying renewable energy technologies will require the application of knowledge, concepts, and tools from a variety of fields including chemistry, materials science, physics and, in particular, electrochemistry. In this presentation we highlight the important achievements in the development of highly active, stable and selective solid-aqueous and solid-organic electrochemical interfaces that will be able to resolve many of the challenging problems related to clean energy production, conversion and storage. A key fundamental issue that will be addressed is the degree to which the fundamental understanding of the synergy between covalent and non covalent interactions can form the basis for any predictive ability in tailor making real world catalysts. We argue that achieving this goal needs a hierarchical strategy to define, at atomic/molecular levels, ever more precisely the potential-controlled bond-making and breaking events that are simultaneously controlled by a the structure and nature of surface atoms, and organization of the electrolyte components that operates in the double layer. The range of materials and electrolytes that will be discussed is broad; involving metals, metal/metal-oxides, pure oxides, S-/N-/C-based materials as well as aqueous electrolytes with a wide pH range, impurity-free organic solvents, and model solid electrolytes. Links between aqueous- and organic-based environments will also be addressed, encouraging the “fuel cell” and “battery” communities to move forward together. We conclude, we are witnessing the renaissance of electrochemistry.

O.S.F.3.

Tailored materials for electrochemical applications

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Electrocatalysis is a subclass of heterogeneous catalysis that is aimed towards increase of the electrochemical reaction rates that are taking place at the surfaces. Real-world electrocatalysts are usually based on precious metals in the form of nanoparticles due to their high surface-to-volume ratio, which enables better utilization of employed materials. Ability to tailor nanostructure of an electrocatalyst is critical in order to tune their electrocatalytic properties. Over the last decade, that has mainly been achieved through implementation of fundamental studies performed on well-defined extended surfaces with distinct single crystalline and polycrystalline structures. Based on these studies, it has been demonstrated that performance of an electrocatalyst could be significantly changed through the control of size, composition, morphology and architecture of employed nanomaterials. This presentation will outline the most important in development of an efficient electrocatalyst: 1) electrochemical properties of well-defined surfaces, 2) synthesis and characterization of different electrocatalysts, and 3) correlation between physical properties (size, shape, composition and morphology) and electrochemical behavior (activity and durability). In addition, a novel research platform in the development of functional nanomaterials for energy conversion and storage applications such as fuel cells electrolyzers and batteries will also be presented.

O.S.F.4.

Nanostructured catalyst engineering towards efficient solar fuel production

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Arising from the global energy demand and climate change, the conversion of greenhouse gas carbon dioxide into value-added chemicals and fuels is attracting increasing commercial attention. The crux for the successful development of this promising technology is the exploration and discovery of highly active, selective and stable catalysts. Herein we demonstrate that the photo-catalytic conversion of CO_2 can be driven by Nb_2O_5 nanorod-supported Pd nanocrystals, without external heating. We also demonstrate that the catalytic activity and selectivity of CO_2 reduction to CO and CH_4 products can be systematically tailored by varying the size of the Pd nanocrystals to achieve a CO production rate surpassing 18.8 mol h^{-1} gPd^{-1} with 99.5% CO selectivity. These performance metrics establish a new milestone at the forefront of catalytic nanomaterials that can enable solar-powered gas-phase heterogeneous CO_2 reduction. The remarkable control over the catalytic performance of Pd@Nb_2O_5 is demonstrated to stem from a combination of photothermal, electronic, and size effects. The insight gleaned from this detailed experimental-theoretical study provides a blueprint for how to tailor the performance metrics of earth-abundant low-cost metal-metal oxide (M@M'Ox) analogues.

O.S.F.5.

On the frontiers of ultra-wide bandgap semiconductors

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Despite the rapid progress in III-nitride-based laser diodes, sub-300 nm UV semiconductor lasers have not been realized mainly due to technical and scientific barriers arising from the lack of proper crystalline substrates and poor understanding of point defect control in wide bandgap semiconductors. While doping is (almost) trivial in classical semiconductors (Si, Ge, GaAs), it becomes increasingly more challenging as the bandgap widens. Excess available energy drives the incorporation of unwanted impurities and generation of native point defects, which act as compensators, resulting in high resistivity and low mobilities. Based on current understanding of point defect energetics, we developed a Fermi level control scheme that suppresses compensation during growth and enables effective n- and p-doping. This point defect control scheme uses photo-generated charge carriers to control the electro-chemical potential of the system and the formation energy of charged point defects.

This point defect control scheme led to devices with much higher efficiency and has a potential to enable the exploitation of AlGaN alloys over the whole composition range (bandgap of 3.4-6.1 eV). These developments have recently resulted in the first demonstration of lasing from a semiconductor at 260 nm.

O.S.F.6.

Exploring nanomaterials synthesis on the length scale of fundamental building blocks

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In this talk I discuss acceleration of materials synthesis using a framework that starts with “breaking down” materials into their fundamental building blocks (FBBs). The M-O bond lengths in octahedrally coordinated MO_6 molecular units capture the interactions that are key to the crystal structure the electronic structure and functionality of materials. Such simple and well characterized units facilitate integration of synthesis, characterization, theory and computation for discovery of general synthesis rules. The example of TiO_2 shows that the distortion of individual octahedral FBBs and their spatial connectivity measured by various experimental techniques and calculated theoretically determines whether a compound with the same stoichiometry will exhibit the properties of anatase, rutile, or some other less common metastable phase. Combining different FBBs with specific functionality is a promising platform for accelerating the pace of discovery of advanced multifunctional materials such as multiferroics, multifunction catalysts, correlated and quantum materials.

O.S.F.7.

Formation mechanism of photovoltaic perovskite nanowires

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Photovoltaic perovskite ($CH_3NH_3PbI_3$) nanowires in association with carbon nanostructures (carbon nanotubes and graphene) make outstanding composites with rapid and strong photoresponse. They can serve as conducting electrodes, or as central components of detectors. Performance of several miniature photo-field effect transistor devices based on these composite structures will be demonstrated.

Then our latest findings on the guided growth of perovskite nanowires by ‘solvatomorph-graphoepitaxy’ will be presented. This method turned out to be a fairly simple approach to overcome the spatially random surface nucleation. The process allows the synthesis of extremely long (centimeters) and thin (a few nanometers) nanowires with a morphology defined by the shape of nanostructured open fluidic channels. A common mechanism underlying of hybrid perovskite nanowire formation will be discussed in detail.

The ‘solvatomorph-graphoepitaxy’ could open up an entirely new spectrum of architectural designs of organometal-halide-perovskite-based heterojunctions -and tandem solar cells, LEDs, photodetectors and new type of magneto-optical data storage devices.

Acknowledgement: The work has been performed in collaboration with Alla Arakcheeva, Andrea Pisoni, Xavier Mettan, Gábor Náfrádi, Osor S. Barišić, Jaćim Jaćimović, Károly Holczer, László Mihály and Claudio Grimaldi. This work was partially supported by the ERC Advanced Grant (PICOPROP#670918).

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O.S.F.8.

Two decades of commercializing nanotechnology for medical devices

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There is an acute shortage of organs due to disease, trauma, congenital defect, and most importantly, age related maladies. Synthetic materials used in medical device and tissue engineering applications today are typically composed of micron sized particles/grains and associate surface roughness. Although human cells are on the micron scale, their individual components, e.g. proteins, are composed of nanometer features. By modifying only the nanofeatures on synthetic material surfaces without changing surface chemistry, it is possible to increase tissue growth of any human tissue by increasing the endogenous adsorption of adhesive proteins (and their bioactivity) onto the material surface. In addition, our group has shown that these same nanofeatures and nano-modifications can reduce bacterial growth without using antibiotics, which may further accelerate the growth of antibiotic resistant microbes. Finally, material nanofeatures have been shown to stimulate the growth and differentiation of stem cells, which may someday be used to treat incurable disorders, such as neural damage. This talk will summarize techniques and efforts to create nanofeatures for a wide range of medical device and tissue engineering applications, particularly those that have received FDA approval and are currently being implanted in humans.

O.S.F.9.

TiO_2 nanocomposites for biomedical applications

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Nanotechnology offers efficient solutions for many areas of science and technology spanning from solar cells to medicine. Owing to rapid development of synthesis and nanofabrication methods we are able to engineer advanced materials at atomic and molecular levels and assemble them into functional devices. Integration of inorganic nanoparticles with soft and biological materials results in one of promising types of hybrids for advancing medical technologies. TiO_2 nanoparticles with their extraordinary stability, exceptional photoreactivity and biocompatibility have a special place in biomedical solutions of the future. Reconstructed surfaces of TiO_2 nanoparticles differ from the bulk by the presence of highly reactive under-coordinated surface. The coordination sphere of the surface metal atoms is incomplete and exhibit high affinity for oxygen-containing ligands what provides the opportunity for their chemical modification. Manipulation of the TiO_2 nanoparticle surface was found to alter the way nanoparticles interact with light and enhance their chemical reactivity and improving their optical properties in the visible region. These ligands were used as "leads" that bridge the electronic properties of semiconductors to electroactive biomolecules such as DNA or proteins. We have utilized monoclonal anti-EGFR antibodies (C225) for targeting of nanoparticles to the epithelial colon cancer cells. Photoinduced charge separation was than employed to create reactive oxygen species and induce apoptosis in the tumor cells. “Cold light,” or bioluminescence, the same property exhibited by fireflies, was also used to develop localized therapy that is activated only in the cancers, leaving healthy cells intact.

O.S.F.10.

2D materials nanosculpting and bioelectronics applications

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Electron beams constitute powerful tools to shape materials with atomic resolution. I will describe experiments that push the limits of device size to atomic scale in 2D materials and expand their function and precision, while addressing fundamental questions about structure and properties at atomic scales. Experiments include fabrication of nanoribbons and field-effect-transistors from novel two-dimensional materials down to sub-nm widths and the ultrafast, all-electronic detection and analysis of biomolecules with nanopores. As molecules are driven through nanopores in solution, they block the ion current flow resulting in current reductions from which molecule’s physical and chemical properties are inferred. DNA, proteins, microRNA and other biomolecules can be analyzed. The temporal, spatial resolution and sensitivity in these experiments have been improved over the last few years thanks to advanced materials, device designs and new electronics.

O.S.F.11.

Calcium phosphate as a key material for socially responsible tissue engineering

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Socially responsible technologies are designed while taking into consideration the socioeconomic, geopolitical and environmental limitations of regions in which they will be implemented. In the medical context, this involves making therapeutic platforms more accessible and affordable to patients in poor regions of the world wherein a given disease is endemic. This often necessitates going against the reigning trend of making therapeutic nanoparticles ever more structurally complex and expensive. However, studies aimed at simplifying materials and formulations while maintaining the functionality and therapeutic response of their more complex counterparts seldom provoke a significant interest in the scientific community. In this talk we demonstrate that designing simple compositions while adopting a rigorous materials science framework of study can be meaningful. As the example, we use osteomyelitis, a disease particularly prevalent in the underdeveloped parts of the world wherein poverty, poor sanitary conditions and chronically compromised defense lines of the immune system are the norm. We show that calcium phosphate nanoparticles, which are inexpensive to make, could be chemically designed to possess the same functionality as a hypothetic mixture additionally composed of: (a) a bone growth factor; (b) an antibiotic for prophylactic or anti-infective purposes; (c) a bisphosphonate as an antiresorptive compound; (d) a viral vector to enable the intracellular delivery of therapeutics; (e) a luminescent dye; (f) a radiographic component; (g) an imaging contrast agent; (h) a magnetic domain; and (i) polymers as viscous components enabling the injectability of the material and acting as carriers for the sustained release of a drug. In particular, calcium phosphates could: (a) produce tunable drug release profiles; (b) take the form of viscous and injectable, self-setting pastes; (c) be naturally osteoinductive and inhibitory for osteoclastogenesis; (d) intracellularly deliver bioactive compounds; (e) accommodate an array of functional ions; (f) be processed into macroporous constructs for tissue engineering; and (g) be naturally antimicrobial. All in all, we see in calcium phosphates the presence of a protean nature whose therapeutic potentials have been barely tapped into.

O.S.F.12.

Graphene research and development: opportunities and challenges

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Graphene and 2D Materials and their derivatives, are slowly moving form academia to industry space becoming more familiar across many industries, entrepreneurs and investors in terms of their superior properties, development of production technologies, processing and new products and devices development.

In this talk, I will review some of the latest developments on graphene research and translation of graphene research to industry applications from our group including environmental, agriculture, protective coatings, sensors, supercapacitors, antennas providing some key challenges and future prospects.

O.S.F.13.

2D dichalcogenide electronic materials and devices

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The discovery of graphene marked the start of research in 2D electronic materials which was expanded in new directions with MoS_2 and other layered semiconducting materials. They have a wide range of promising potential applications, including those in digital electronics, optoelectronics and flexible devices. Combining 2D materials in heterostructures can increase their reach even further.

In my talk, I will present our recent efforts in growing 2D semiconducting transition metal dichalcogenides (TMDCs) and heterostructures using a variety of techniques such as CVD and MBE, starting from epitaxial growth of MoS_2 on sapphire with a high degree of control over lattice orientation. Next, I will show our work on atomically thin rhenium disulphide (ReS_2) liquid-electrolyte gated transistors with atypical behaviour at high charge densities related to the peculiar band structure of this material. I will finish by presenting new results on spin/valley transport in semiconducting monolayer TMDC materials.

O.S.F.14.

Nanopores in 2D materials - opportunities and challenges

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Atomically thin nanopore membranes are considered to be a promising approach to achieve single base resolution with the ultimate aim of rapid and cheap DNA sequencing. Recently, we made advances in using nanopore platform for its integration with 2D materials such as graphene or MoS_2. Translocation of various types of DNA exhibits a signal amplitude that is five times higher than in the case of solid-state Si_3N_4 membranes and a SNR of more than 10. Although single nucleotide identification and DNA sequencing using biological pores have already been demonstrated their fragility, difficulties related to measuring pA-range ionic currents together with their dependence on biochemical reagents, make solid state nanopores an attractive alternative. In this talk I will address novel applications that address identification of single nucleotides but as well go beyond DNA sequencing. We use novel solid state nanopore platform based on atomically thin nanopore membranes in 2D materials such as graphene or molybdenum disulfide for DNA detection, sequencing, water desalination and osmotic power generation.

PL.S.V.1.

From MAX to MXene - From 3D to 2D

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By now it is well-established that the layered, hexagonal carbides and nitrides with the general formula, Mn+1AXn, (MAX) where n = 1 to 3, M is an early transition metal, A is an A-group (mostly IIIA and IVA) element and X is either C and/or N – sometimes referred to as polycrystalline nanolaminates because every basal plane is a potential deformation or delamination plane - combine some of the best attributes of metals and ceramics. More recently we showed that by simply immersing MAX phase powders, at room temperature, in HF or HCl and LiF solutions, the A-layers – mostly Al - are selectively etched to produce 2D materials that we labeled MXenes to emphasize the loss of the A-group element and their similarities to graphene. Unlike hydrophobic graphene, MXenes are hydrophilic and behave as "conductive clays", a hitherto unknown combination. MXenes such as Ti_2C, V_2C, Nb_2C and Ti_3C_2 can be used as electrode materials in lithium-ion batteries (LIBs) and supercapacitors (SC) as well as transparent conductive electrodes, with performances that are quite impressive. In all cases, when used as anodes in LIB, MXenes showed an excellent capability to handle high cycling rates. Flexible, additives-free electrodes of delaminated Ti_3C_2 showed reversible capacities of > 400 mAhg-1 at 1 C and 110 mAhg-1 at 36 C, the latter for > 700 cycles. SC's with volumetric capacitances of > 1100 F/cm^3 have been obtained. The potential of using MXenes – possibly the largest family of 2D materials known with > 20 members and with new ones being discovered almost monthly - as transparent conductive electrodes, electromagnetic shielding, water remediation, among many other applications will be highlighted.

PL.S.V.2.

Atomically resolved interfacial coupling and polarization of ABO_3 heterostructures

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Interfaces with subtle difference in atomic and electronic structures in perovskite ABO_3 heterostructures often yield intriguingly different properties, yet their exact roles remain elusive. In this presentation, we report an integrated study of unusual transport, magnetic, and structural properties of $Pr_{0.67}Sr_{0.33}MnO_3$ films and $La_{0.67}Sr_{0.33}MnO_3$ films of various thicknesses on $SrTiO_3$ (STO) substrate. In particular, using atomically resolved imaging and electron energy-loss spectroscopy, we measure interface related local lattice distortion, BO_6 octahedral rotation and cation-anion displacement induced polarization. In the very thin $Pr_{0.67}Sr_{0.33}MnO_3$ film, an unexpected interface-induced ferromagnetic polaronic insulator phase was observed during the cubic-to-tetragonal phase transition of STO, due to the enhanced electron-phonon interaction and atomic disorder in the film. For the very thin $La_{0.67}Sr_{0.33}MnO_3$ films we reveal a remarkably deep polarization in non-ferroelectric STO near the interface due to its build-in electric field. Combining the experimental results including electron holography with first principles calculations, we propose that the observed deep polarization and field are originated from oxygen vacancies that extend beyond a dozen unit-cells from the interface, thus providing important evidence of the role of defects in the emergent interface properties of transition metal oxides. The work was supported by DOE-BES-MSE under Contract DE-AC02-98CH10886. Collaborations with L. Wu, B. Zhang, G. M. Chow, Z. Wang, J. Tao, L. Yu, M-G. Han, J. Zhang, and E. W. Plummer are acknowledged.

PL.S.V.3.

Half-Heusler spinodal thermoelectrics with high ZT

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Hitherto non-centrosymmetric multi-component half-Heusler phases have proven to be excellent thermoelectrics which are able to efficiently convert waste exhaust heat of internal combustion engines into electricity. Large-scale production and particularly nanostructuring of Half Heusler-based thermoelectric materials by preferably system-inherent phases need a profound knowledge not only of isothermal phase relations, temperature dependent solubilities but also of the solidification behavior.

The current presentation will cover a detailed description of the state of art of research on Half-Heusler thermoelectrics leading to optimised >98% dense bulk TE-material with ZT-values (ZT = figure of merit) reaching ZT = 1.4 for p-type grades and ZT = 1.5 for n-type grades. The presentation will focus on a detailed experimental investigation (backed by SEM/TEM analyses, DFT) of the constitution of the {Ti,Zr}-Ni-Sn systems including a liquidus projection and a Scheil diagram, as well as a CALPHAD calculation. For the binary systems TiNiSn-ZrNiSn and TiNiSn-HfNiSn, thermodynamic spinodal/binodal curves as well as coherent spinodal demixing (nanostructuring of thermoelectrics) have been determined from solubility data and DFT calculations.

Although among $Ti_{1-x-y}Zr_xHf_yNiSn_{1-z}Sb_z$ compounds the thermoelectric behavior reached ZT ~ 1.5 at 850 K, we reached already a ZT~1.2 for Hf-free n-type $Ti_{0.5}Zr_{0.5}NiSn_{0.98}Sb_{0.02}$ and {Ti,Zr,Nb}Ni $Sn_{0.98}Sb_{0.02}$ yielding an thermoelectric efficiency of ~ 11%. These excellent TE data prove that Hf-free and therefore cheap half-Heusler alloys can be promising materials for a large scale production route.

PL.S.V.4.

Nanomagnetism: Superparamagnetism in iron - doped CeO_2-y nanocrystals

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Magnetic properties of materials fundamentally change when the particle sizes are reduced [1]. Below a critical size (DC), which typically lies below 100 nm, normal microscopic multidomain ferromagnetic (FM) structure is energetically unfavorable, and the particles are in single domain state. In this state, the mechanism of magnetization reversal can only occur via the rotation of the magnetization vector from one easy magnetic direction to another over the magnetic anisotropy barrier [2]. As particle size decreases within the single domain range, another critical threshold (DSP) is reached, at which remanence and coercivity go to zero and the particles are in the superparamagnetic (SP) state. Such a system has no hysteresis and magnetization curves at different temperatures superimpose onto a universal curve of M/MS vs H/T (Langevin's curve). We have measured the magnetization of undoped and $Fe^{2+/3+}$ doped CeO_2-y nanocrystals at various temperatures and magnetic fields [3]. In the case of Fe-doped samples, the superparamagnetic behavior of this system is revealed by nearly zero coercive field, an appearance of the blocking temperature below 20 K, as well as the M(H) dependence, which is well fitted by weighted Langevin function which takes into account particle magnetic moment distribution [3].

We have also measured Raman scattering spectra of these nonocrystalline samples. Raman mode exhibits softening and broadening by changing the valence state of Fe dopant, as a consequence of the electron-molecular vibration coupling. The electron-molecular vibration (phonon) coupling constants λ and density of electron states at the Fermi level per spin and molecule N(0)=22 (eV)-1 were determined. The Stoner condition N(0)I>1 is multiple fulfilled in the case of nano CeO_2-y favoring the band ferromagnetism approach [4].

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PL.S.V.5.

Tailoring epitaxial oxide thin film on Si(001) using pulsed-laser deposition

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Epitaxial integration of transition metal oxides with semiconductors brings a great number of exciting electrical, magnetic, and optical properties to the well-established silicon platform and represents a milestone for many novel device applications. A convenient way of integrating functional oxides with Si(001) substrate is through a $SrTiO_3$ (STO) intermediate layer, which has been grown in epitaxial form and with high crystallinity using molecular beam epitaxy (MBE) mainly. However, run-to-run stability of the MBE deposition process and difficult stoichiometry control makes this method inappropriate from an industrial point of view.

In this work we focused on the possibilities of using the pulsed-laser deposition (PLD) technique for the synthesis of functional layers on Si(001), as an alternative manufacturing route compared to MBE. First, metallic strontium was used to prepare (1×2)+(2×1) reconstructed Sr(1/2 ML)/Si(001) surface, which serves as a buffer material and hinders intense reaction of the constituents. For successful Si passivation unique structural analysis of the surface using Low Energy Electron Diffraction, Scanning Tunneling Microscopy, and X-ray Photoelectron Spectroscopy was introduced. Subsequently, detailed analysis of STO initial deposition parameters was performed, which enabled us to develop a complete protocol for integration, taking into account the peculiarities of the PLD process. The as-prepared oxide layer exhibits STO(001)||Si(001) out-of-plane and STO[110]||Si[100] in-plane orientation. In the final stage, piezoelectric $Pb[Mg_{1/3}Nb_{2/3}]O_3$-$PbTiO_3$ (PMN-PT) layer was integrated with as-prepared template. Due to its giant piezoelectricity in the thin film form PMN-PT represents a prime candidate for the active layer in microelectromechanical systems (MEMS), which integration with Si will also be discussed in the presentation.

O.S.I.1.

Mechanical properties of high efficiency thermoelectric materials (skutterudites, half Heusler alloys and clathrates)

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Skutterudites, half-Heusler alloys and clathrates are known as promising candidates as leg materials for thermoelectric generators, which can directly convert waste heat into electricity; they are environmentally friendly, can be used in a wide temperature range and the starting material is available and cheap.

In this paper we show our latest p- and n-type skutterudites, Hf-free half-Heusler alloys and clathrates with high ZT values and high efficiencies.

A prerequisite for commercial use is mechanical robustness to undergo repetitive thermo cycling and to resist cracking or failure from any vibration. For these reasons, various mechanical properties and their dependence on density and hardness have been evaluated.

Concerning modules, built with p- and n-type materials, it is of importance to know the exact thermal expansion coefficient of each material in the temperature range the module is used. An overview of all our data in comparison with other thermoelectric materials will be given.

O.S.I.2.

Plasma electrolytic oxidation of TA6V for the improvement of its surface hardness

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Plasma Electrolytic Oxidation (PEO) is an innovating high-energy electrochemical process, used to coat light materials, i.e. aluminum, titanium or magnesium alloys, in order to improve their surface properties. These processes are environmentally-friendly and enable the growth of films usually thicker than films obtained with similar processes (like anodisation).

This work is focused on Ti-6Al-4V, a titanium alloy that possesses excellent thermal and mechanical properties but whose surface tribological behaviour needs substantial improvements. Coatings have been here prepared by PEO process, using Bipolar pulsed DC mode.

We have managed to prepare coatings of varying thicknesses, depending on process parameters, in several electrolyte media. The roughness and porosity of the coatings vary both as a function of the electrolyte's composition. All these characteristics have a significant impact on micro-hardness measurements. Nevertheless, in appropriate conditions, coatings with improved hardness, with respect to the substrate, were obtained.

O.S.I.3.

Structural investigation of the AZ61 Magnesium alloy, in dependence of various heat treatment processes, TEM analyze

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Precipitation phases created in the microstructure of Mg-Al-Zn AZ61 Magnesium workable alloy, in dependence of heat treatments process regimes: solution heat treatment in temperatures 4700C for 5 hours and precipitation heat treatment in temperatures 1000C, 1500C, 2000C, 2500C, 3000C in 1h and 15h, were examined in this study. Through this regimes in the AZ61 alloy microstructure by TEM-EDX analyzes are effectuated these precipitations phases Al-Mn, Al4Mn, Al_8Mn_5, Mg-Si, Al-Mg-Mn. Light Microscopy after this regimes and controlling methods, distinguished and demonstrate precipitations particles phases of Al-Mn, Mg-Si, Al-Mg-Mn, Al-Mg-Si, Al-Mg-Si-Mn, Al-Mg-Mn-Fe, Al-Mg-Si-Fe with size 0.3 μm – 50 μm, by having morphology of disc, needle, plate and rounded shape. Quantitative analyze of volume fraction by light microscopy, under the regime of temperature 1000C for 1h and 15h has effectuated the highest volume fraction of precipitation particles.

O.S.I.4.

Application of new modifier CaSiBa containing barium during production of low alloy steel

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The aim of this article is focused on evaluation of new experimental modifier CaSiBa during production of low alloy steel. The alloy containing approximately 15 % of barium and the same amount of calcium was used like a deoxidation agent. According to the physical-chemical properties, both alkaline earth metals have high affinity to oxygen and sulphur and also ability to modify inclusions in steel into globular shape. These proper attributes should contribute to the improvement of steel mechanical properties. Two experimental almost 50 kg melts were carried out – the first one modified as usual by aluminium and the second one by CaSiBa alloy. The influence of modification by barium was mainly evaluated by SEM, EDAX, determination of content of non-metallic inclusions and change of mechanical properties.

O.S.I.5.

Influence of the type of substrate rotation on microstructure of magnetron sputtered nanolayered TiAlN/TiSiN coatings

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In industrial coating deposition systems substrates move in a planetary-like manner to ensure uniform coating deposition on all surfaces. In this study, influence of the type of substrate rotation on phase composition, crystal orientation, microstructure and surface morphology of nanolayered TiAlN/TiSiN coatings was investigated. Scanning electron microscopy, transmission electron microscopy, atomic force microscopy, X-ray photoelectron spectroscopy, X-ray diffraction and nanoindentation technique were applied for coating characterization. It was found that the type of rotation greatly influences both crystal orientation and microstructure. Coating prepared with single rotation was of columnar and porous microstructure with crystallites oriented in 111 and 200 directions. Conversely, there were no signs of columnar growth for coatings prepared with double and triple rotations which were of compact and dense microstructure with crystallites oriented in 200 direction. As a result, coatings prepared with higher number of rotations were smoother and of considerably higher hardness.

O.S.I.6.

Synthesis and thermal stability of immiscible metal (Au–Rh, Au–Ir, Au–Ir–Rh and Pd-Rh) nanoalloys

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The report highlights synthetic approach to the preparation of nanoalloys of immiscible metals based on thermolysis of single-source precursors. We successfully prepared nanoalloys in the systems of Au–Ir, Au–Rh, Au–Ir–Rh and Pd-Rh with large bulk miscibility gaps, in one-run reactions under thermal decomposition of specially synthesised double-complex salts $[AuEn_2][Ir(NO_2)_6]$, $[AuEn_2][Ir(NO_2)_6]x[Rh(NO_2)_6]_{1-x}$, $[AuEn_2][Rh(NO_2)_6]$, $[Rh(NH_3)_5Cl][Pd(NO_2)_4]$, $[PdEn_2]_3[Rh(NO_2)_6]_{2\cdot 2.67}H_2O$ and $[RhEn_3]_2[Pd(NO_2)_4]_3$. The TEM microscopy observations show that the nanoalloy structures are composed of well-dispersed aggregates of crystalline domains with a mean size of 5±3 nm. EDX analysis and XRD measurements confirm the formation of AuIr, AuRh, AuIrxRh1-x, PdxRh1-x metastable solid solutions. In situ high-temperature synchrotron XRD was used to study the formation mechanism of nanoalloys. The obtained metastable nanoalloys exhibit essential thermal stability. Exposure to 180 ºC for 30 h does not cause any dealloying process.

The work has been supported by grant of Russian Science Foundation (project №16-13-10192).

O.S.II.1.

Synthesis, processing, thermal and luminescence properties of Eu^{3+} -doped Gd_2O_3 powders

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Nanometric-sized pure and Eu^{3+} -doped gadolinia (Gd_2O_3) powders were obtained by applying solid-state displacement reaction at low temperature. The XRD analysis revealed that the room temperature product was gadolinium hydroxide, $Gd(OH)_3$. In order to induce crystallization of Gd_2O_3, the subsequent calcination at 600-1200°C of the room temperature reaction products was studied. The pure cubic Gd_2O_3 phase was made at 600°C which converted to monoclinic Gd_2O_3 phase between 1400° and 1600°C. High-density (96% of theoretical density) ceramic pellet free of any additives was obtained after pressureless sintering at 1600°C for 4 h in air, using calcined powder at 600°C. The room temperature thermal diffusivity as well as calculated thermal conductivity of Gd_2O_3 sample sintered at 1600°C for 4 h in air showed the average value of 1.33 mm2/s and 7.4 W/(m×K), respectively. Five bands associated with 5D0-7FJ (J=4, 3, 2, 1 and 0) spin forbidden f–f transitions can be observed. It is found that emission spectra depend on Eu^{3+} concentration. Emission spectrum for 5% of Eu^{3+} represents Eu^{3+} luminescence in monoclinic matrix, and for 0.5% of Eu^{3+} concentration we can observe Eu^{3+} luminescence in cubic phase of Gd_2O_3. Transition from cubic to monoclinic phase of Gd_2O_3 with change of dopant concentration is studied.

O.S.II.2.

Interrelations between positive and negative coercive fields of ferroelectric domains measured by variable amplitude cycling

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Ferroelectric materials are used for a wide range of modern microelectronics applications, especially memory devices. Understanding a switching behavior in these materials characterized by coercive electric fields plays a significant role in the engineering of such devices. The joint distribution function of ferroelectric coercive fields in PZT-based capacitors is measured by running linear-sweep cyclic voltammetry with a progressively changing maximum voltage. In this approach, the correlation degree of positive and negative coercive fields is estimated based on the changes in the negative peak of current-voltage curves with each step of the maximum cyclic voltage scanning the positive peak. As at each maximum voltage step a different number of ferroelectric domains changes their polarization, the changes in the negative peak provide the distribution of negative coercive fields for the domains with a known value of the positive coercive field. It is found that correlations between the positive and negative coercive fields are smaller than one would expect from the symmetric model of ferroelectric switching. We have also observed a peak-splitting effect and identified some of its features. The suggested approach of determining the joint distribution function is general and thus can be applied to other materials and devices.

O.S.II.3.

Synthesis and characterization of $Li_2FeP_2O_7$ cathode material

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The search for alternative cathode materials for Li-ion batteries has recently emerged $Li_2FeP_2O_7$ pyrophosphate as a new potential competitor for $LiFePO_4$ material. It has a possibility to offer good rate capability, lithium ion diffusivity and volumetric energy density, and is a material of high safety and low raw materials cost. In addition, there is the probability of releasing the second Li-atom at a higher redox potential of 5.2 V, where the theoretical capacity would reach 220 mAhg−1. Optimized solid state reaction is used for the synthesis of pure $Li_2FeP_2O_7$ powder and a composite $Li_2FeP_2O_7$/C. The synthesized powders are characterized by X-ray powder diffraction, field emission scanning electron microscopy, FTIR spectroscopy, and galvanostatic charge/discharge cycling.

O.S.II.4.

Preparation, modification and application of multi-layered MXene structures in gas sensors

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Since the discovery of graphene, one can observe growing trend toward preparation of two-dimensional (2D) nanomaterials featured by unique properties and wide spectrum of potential applications. Among the others, one of the most intensively investigated 2D nanomaterials are freshly discovered transition metal carbides or nitrides called MXenes.

The MXene structures are derived from ternary metal ceramic alloys called MAX phases, where M - transition metal, A - 13 or 14 group compound and X - C and/or N. The removal of A layer via chemical etching, leads to the formation of multi-layered, quasi 2D, accordion like structures. The subsequent intercalation and delamination of multilayered MXenes allow obtaining single-layered graphene like nano-sheets.

Nowadays, most of the research is focused on the application of multi-layered MXene powders. Thanks to their high specific surface area, it is believed they are excellent candidates for electrode material in energy storage systems. Another promising direction pointed by theoretical research is resistive gas sensors.

In this work, we present the results of experimental research related to the application of multi-layered MXenes as an active component in resistive gas sensors. Ti_3C_2 MXenes were derived from Ti_3AlC_2 MAX phases via hydrofluoric acid treatment. Parental 312 MAX phase sinter was prepared via volume combustion synthesis method from powder mixture of TiC and Ti_2AlC MAX phase. Part of MXene sample additionally underwent chlorosulfonic acid treatment. As prepared samples were deposited onto commercially available interdigitated gold electrodes via drag and drop method or by poly(3,4-ethylenedioxythiophene) assisted electro-deposition process. It was found that sensor selectivity toward ammonia or nitrogen dioxide was dependent on MXene modifications. Moreover, MXene based sensors were highly resistant to environmental humidity.

This work was financially supported by the National Science Centre of Poland (SONATA 7 programme, 2015-2018, grant No. 2014/13/D/ST5/02824.

O.S.II.5.

Tuning electronic properties of MoS_2 by doping nonisovalent niobium and rhenium ions

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Molybdenum disulfide, because of its electronic properties, can find wide application in photocatalysis, as cathode material of Li-ion batteries, in optoelectronic sensors and so on. By modifying MoS_2 with doping impurities, materials with a variety of electronic properties can be obtained.

This work is devoted to investigation of molybdenum disulphides doped with rhenium atoms (electronically abundant compared to molybdenum atoms) or niobium (electronically deficient compared to molybdenum atoms) by high-energy spectroscopy methods. These methods make it possible to study in detail the changes in the electronic structure as a result of the introduction of dopant atoms into the structure of MoS_2. Obtained data were compared with magnetic measurements.

The work was supported by the Russian Science Foundation (Grant no. 14-13-00674).

O.S.II.6.

Enhanced natural sunlight- and artificial UV-driven photocatalytic activity of mechanically activated ZnO/SnO_2 composite

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Over the past four decades there is an increasing interest to develop highly efficient semiconductor photocatalysts for degradation of organic and biological pollutants in water under light irradiation. The semiconductor band gap determines which wavelength of light will be absorbed; precisely, semiconductors with a wide band gap (> 3 eV) can absorb only UV light, while those with a narrow band gap (< 3 eV) can be activated by visible light.

In this study we examined structural, morphological, textural and optical properties of ZnO/SnO_2 composite as potential photocatalyst. Mechanical activation of commercial ZnO and SnO_2 powders has been used to produce a composite with high density of surface defects. To investigate the influence of thermal treatment on the physical properties, and consequently on photoactivity, the composite has been additionaly annealed at 400 and 700 °C. The phase purity, crystal structure and average crystallite size of pristine metal oxides and the composites were investigated by X-ray diffraction and Raman spectroscopy. The particles morphology and size distributions were studied by FE–SEM and laser diffraction particle size analyzer, respectively. The textural properties were determined from N¬2¬ adsorption/desorption experiments, while the optical properties were studied using UV–Vis diffuse reflectance and photoluminescence spectroscopy. Photocatalytic activity of pristine ZnO and ZnO/SnO2 composites were examined via de-colorization of methylene blue under: (1) direct natural sunlight, and (2) artificial UV irradiation. In both cases enhanced photocatalytic activity of ZnO/SnO_2 has been found. Enhanced photocatalytic activity can be attributed to the surface defects and to created ZnO/SnO_2 heterojunctions which reduced electron-hole recombination time.

O.S.III.1.

Highly selective anticancer activity of core shell particles based on hydroxyapatite, chitosan lactate and different androstane derivatives

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Hybrid systems based on nano hydroxyapatites (HAp) are the subject of numerous studies in preventive and regenerative medicine. Special interests are directed towards the creation of a system based on HAp for use in a nano-oncology. The main objective of this research is directed towards the creation of a system with cytotoxic properties towards the cancer cells with the same time, minimum side effects. Carriers base on core shell of HAp/chitosan-poly(D,L)-lactide-co-glycolide (PLGA) loaded with androstane-based cancer inhibitor could be seen as promising drug delivery platforms for selective cancer therapies.

In this study we utilize an emulsification process and freeze drying to load the composite particles based on HAp nanocarrier, chitosane (Ch), PLGA and chitosan oligosaccharide lactate (ChOL) with 17β-hydroxy-17α-picolyl-androst-5-en-3β-acetate (A) and 3β,17β-dihydroxy-16-hydroxymino-androst-5-en (B), a chemotherapeutic derivatives of androstane. The picolyl androstane derivatives showed high potency in the cell inhibitors of hormone-dependent cancers (lung, prostate and colon cancer; adeno and cervix carcinoma; etc.).

1H NMR, 13C NMR and high-resolution time-of-flight mass spectrometry (MS) techniques confirmed the intact structure of the derivatives A and B. The thermogravimetric and differential thermal analysis (TGA, DTA) coupled with mass spectrometry was used to qualitatively confirm the drug loading process. FT-IR, XRD, AFM and DSC techniques have confirmed the success of androstane (A and B) loading process in core shell particles base on nano hydroxyapatite. All the synthesized particles were found to be spherical in shape with a uniform size distribution from d50=167 to d50=231 nm. Highly selective anticancer activity was noted towards the human lung carcinoma (A549) by A loaded HAp/Ch-PLGA and towards the human breast adenocarcinoma (MDA-MB-231) by B loaded HAp/ChOL. The obtained results of the DET and MTT tests were in agreement.

O.S.III.2.

The atomic-scale defects at the surface of MgO particles and their antibacterial applications

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MgO exhibits a contact-based antibacterial activity. There is a discrepancy in opinions about the impact of atomic-scale surface features on its antibacterial activity. We thoroughly investigated the nature and abundance of native surface defects of four MgO powders from different origin by means of multi-method approach (e.g. photoluminescence, UV/Vis reflectance, infrared spectroscopy and thermogravimetric analysis). Their impact on the hydrolysis kinetics, antibacterial activity and ROS generation potential was determined. The results proved that reduction in abundance of low coordinated oxygen atoms at the surface of MgO improves its resilience against hydrolysis and antibacterial activity. The ROS generation potential was not inherent property of the studied MgO powders, but was rather a side product of hydrolysis and/or a consequence of MgO/bacteria interaction. In this contribution, mutual correlations of hydrolysis, antibacterial activity and ROS generation will be discussed and implications to the mechanism of MgO antibacterial activity will be highlighted.

O.S.III.3.

Design and evaluation of biocompatible 90Y-labeled phosphonate-coated MNPs for possible applications in cancer therapy

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Radiolabeled magnetic nanoparticles coated with hydrophilic phosphonates ligands: imidodiphosphate (IDP) and inositol hexaphosphate (IHP) were developed as multifunctional vectors to localize both radioactivity and magnetic energy at the tumor site. The coating of MNPs with phosphonates increased their colloidal stability and prevented agglomeration, allowed the binding of the radionuclide 90Y for the functional groups on the surface of MNPs and increased the stability of MNPs in vivo. The specific power absorption of MNPs are found to be 46-81 W/g in different physiological media such as phosphate buffered saline (PBS) and saline (NaCl), and their values are suitable for hyperthermia treatment of cancer under an alternating current (AC) magnetic field. The characterized biocompatible MNPs were labeled with radionuclide 90Y in high yield (>98 %) and showed high in vitro and in vivo stability. Since both 90Y-labeled MNPs exhibited favorable properties, they could be promising for the potential use in the combined radiotherapy-hyperthermia cancer treatment.

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O.S.III.4.

Hierarchical self-assembly of highly water-soluble fullerene derivatives

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The unique carbon allotrope family known as the fullerenes boasts many desirable properties for future medical applications, such as antioxidants, photodynamic therapy (PDT) agents and magnetic resonance imaging (MRI) contrast agents. In order to enter the body safely, these highly hydrophobic cages must first be functionalised to increase their water solubility. We have covalently attached ethylene glycol units to fullerene cages of different sizes to yield highly water-soluble derivatives. Precise structural elucidation of these molecules is far from trivial, however, they display some intriguing photoluminescent properties with potential value for fluorescent imaging within the body. Most striking though is our observation that some of these derivatives spontaneously self-assemble over a prolonged period in aqueous solution into hydrogels with complex hierarchical structure. We have characterised these structures with optical and scanning electron microscopies (SEM) and are investigating their utility as novel biomedical materials.

O.S.III.5.

Networks of welded silver nanowires as transparent electrodes

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For their ease and cost-effectiveness of synthesis and processing, silver nanowires (AgNWs) have been extensively studied as a transparent electrode alternative to conventional solutions like indium tin oxide (ITO) for the application in optoelectronic devices like solar cells. In this study, AgNWs were synthesized by a simple polyol reduction process. The main focus of this research was elucidating the solid-state wetting and welding mechanisms that occur during annealing of AgNWs before a layer of aluminum doped zinc oxide (AZO) is deposited on them, for the enhancement of properties essential for an electrode in a solar cell. Microstructural characterization using scanning electron microscopy (SEM) and scanning transmission electron microscopy (STEM) revealed that solid-state wetting and subsequent welding occurred only between nanowires whose contact geometry is characterized by an enormous difference in radii of curvature. Results also indicated that, during annealing, the AgNW in contact through a smaller radius of curvature dissolves, Ag atoms diffuse and are incorporated in a welded zone between the AgNWs whose crystallographic orientation is inherent from the AgNW in contact through a large radius of curvature. Wetting angle between two welded AgNWs was measured to be below 4.8°, indicating almost complete wetting. Tomography, based on 3D reconstruction of STEM imaging, was employed to better understand the morphology of the welded zone and geometric relationship between the AgNWs. Electron diffraction orientation and strain mapping were performed in order to elucidate possible strain fluctuation across the AgNWs. Crystal lattice distortion, directly measured by atomic column displacements in drift corrected cross-sectional atomic resolution STEM images of an AgNW, prepared by focused ion beam (FIB), demonstrated non-uniform distribution of strain in five twin segments of the AgNW. It has been demonstrated that welding of AgNWs significantly reduces electrical resistivity while preserving high optical transparency, properties essential for transparent electrodes utilized in solar cells.

O.S.III.6.

Properties of organic conjugated molecules sensitized by fullerenes

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Optical and nonlinear optical properties of organic material sensitized by carbon nanoparticles were considered in the present paper. The medium with carbon nanoparticles can be applied in the laser radiation modulators and switchers due to their nonlinear optical effects, i.e. nonlinear absorption and high-frequency Kerr effect. It was demonstrated the formation of intermolecular charge transfer complex between donor part of organic molecule and strong nanocarbon acceptor. This intermolecular complex influence on the changes of optical characteristic, for example, transmittance increase of liquid crystal cells was shown. The ability to apply considered molecular system for analysis of bio-objects was demonstrated in the paper as well.

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).

O.S.III.7.

Organic-ligand-assisted hydrothermal synthesis of tailor-made ceramic nanocrystals towards bio-medical applications

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To fine-tune the properties of ceramics, they can now be processed into uniform-size nanocrystals with spherical, cube, sheet, rod, wire shapes. Despite these recent advances, controlling the shape, crystal structure, and surface characteristics of ceramic nanocrystals is still a difficult task. Here, we report an approach to tailor-made ceramic nanocrystals, e.g., anatase TiO_2 nanosheets [1] by means of organic ligand-assisted hydrothermal synthesis towards bio-medical applications [2].

[1] Z. Tan, K. Sato, S. Takami, C. Numako, M. Umetsu, K. Soga, M. Nakayama, R. Sasaki, T. Tanaka, C. Ogino, A. Kondo, K. Yamamoto, T. Hashishin, and S. Ohara, "Particle Size for Photocatalytic Activity of Anatase TiO_2 Nanosheets with Highly Exposed {001} Facets", RSC Advances, 3, p.19268-19271, (2013).
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O.S.III.8.

Small-angle scattering of non-convex nanoparticles: The case of a cube, possessing a rectangular indent

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Small-angle scattering (SAS) is an experimental method for the investigation of nanometric particles.

SAS scattering patterns of many single homogeneous particles have been determined. Such mathematical investigations are of practical relevance. These investigations are indispensable, in order to compare experimental scattering curves Iexp(q) with theoretical ones I(q). This is illustrated in the textbook by W. Gille, Particle and Particle Systems Characterization, SAS Applications, CRC press 2013. For more details see https://www.crcpress.com/Particle-and-Particle-Systems-Characterization-Small-Angle-Scattering-SAS/Gille/p/book/9781466581777.

Section 2 (pages 59-94) explains the concept of the chord length distribution of a particle. The strategy of comparing theory and model in real space has some advantages. However, analytic results of the SAS correlation function (CF) gamma(r) for non-convex particles are relatively rare - sometimes complicated. O. Glatter and O. Kratky have emphasized this in their textbook: Small-Angle X-Ray Scattering, Academic Press, London 1982:

"Thus, the chord length distribution is equally well suited to represent a particle with respects to its diffraction pattern ...". However, there are serious difficulties for non-convex particles and particles with hollow parts.

There exists a basic formula by S. Ciccariello (2005): It describes the connection between the spatial CF gamma(r) of a right cylinder of height H and the CF beta(r) of the base of the cylinder. Based on this, the case of an indented cube (IC) is studied. Analytic expressions for all functions, relevant in SAS, are explained. This includes the interpretation of the signed chord length distribution of the IC.

O.S.III.9.

Au hollow cylindrical nanostructures as optical tunable nanoresonators

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The optical response of Au hollow cylindrical nanostructures with very thin walls (nanocups) has been studied by means of finite difference time domain (FDTD) simulations, which show that, by changing their geometry, they behave as tunable optical nanoresonators with strong near-field enhancement. [1]

According to the simulations, nanostructures of about 400 nm in diameter and height, and a wall and base thickness of about 30 nm, demonstrate a great enhancement of the electromagnetic field inside the cavity, which is promising for fabricating functional devices based on surface-enhanced Raman spectroscopy. Besides, the response of these nanostructures can be tuned along the visible-NIR by changing their geometry.

To obtain these structures, a process combining the concepts from stencil and nanoimprint lithography (NIL) has been used. [2] The key of the process relies on the use of an intermediate hard mask that allows decoupling of the imprint process from the height of the nanostructures, overcoming this way the high aspect ratio limitations of NIL. In brief, this low-cost and easily scalable fabrication route, offers a thorough control of the geometrical parameters, precise position control over the substrate, and easy change of composition, including the possibility to obtain multishell nanocups. FTIR measurements have been performed confirming the simulations results.

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O.S.III.10.

Process development for reproducible synthesis of magnetic eco-friendly adsorbent

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Magnetic particulate adsorbents offer advantages over traditional ones due to facile separation from the aqueous phase. Their efficient removal in magnetic field, followed by re-generation and re-use decreases the overall water treatment cost by eliminating time and energy required for filtration/centrifugation processes. A relatively simple procedure to produce magnetite/chitosan composite (MCC) microparticles has been previously developed by our team and the novel material has demonstrated superior adsorption properties towards some heavy metal ions compared to similar products described in the literature. The use of chitosan as a raw material has multiple advantages, but its structure and properties may vary widely due to the fact that the macromolecules are actually copolymers containing both acetylglucosamine and glucosamine sequences of various lengths. This work aims to investigate the influence of the raw material (chitosan) characteristics upon the MCC properties and to identify the appropriate changes in the synthesis parameters that ensure product reproducibility.

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O.S.III.11.

The slag based adsorbents for Cu^{2+} removal from aquatic solutions

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This study aims to understand the kinetic, thermodynamic and mechanism of Cu^{2+} adsorption onto unmodified electric arc furnace slag (EAFS) and alkali modified EAFS. The adsorption process was investigated via a batch reactor system. The modified EAFS sample has been prepared by reacting an EAFS powder with an aqueous alkali silicate solution. The both samples were characterized by SEM, XRD, FTIR and porosimetric measurements.

The results have shown that alkali activation of EAFS favour adsorption process. The adsorption reaction on both adsorbents was found to be pseudo second order. Thermodynamic investigations have shown that adsorption process is spontaneous and endothermic. Mechanism of adsorption was investigated using the intraparticle diffusion and Boyd model which suggested that the both, film diffusion and diffusion within the pores of adsorbent controls the intraparticle diffusion of Cu^{2+} onto and EAFS and modified EAFS and was mainly due to external mass transport. Besides, FTIR spectroscopy determined the surface functional groups of the EAFS and modified EAFS which participate in Cu^{2+} bonding.

O.S.IV.1.

Particle morphology effects in random sequential adsorption

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The properties of the random sequential adsorption of objects of various shapes on a two-dimensional triangular lattice are studied numerically by means of Monte Carlo simulations. The depositing objects are formed by self-avoiding lattice steps, whereby the size of the objects is gradually increased by wrapping the walks in several different ways. The aim of this work is to investigate the impact of the geometrical properties of the shapes on the jamming density \theta_j and on the temporal evolution of the coverage fraction \theta(t). Our results suggest that the order of symmetry axis of a shape exerts a decisive influence on adsorption kinetics near the jamming limit \theta_j. The decay of probability for the insertion of a new particle onto a lattice is described in a broad range of the coverage \theta by the product between the linear and the stretched exponential function for all examined objects. The corresponding fitting parameters are discussed within the context of the shape descriptors, such as rotational symmetry and the shape factor (parameter of nonsphericity) of the objects. Predictions following from our calculations suggest that the proposed fitting function for the insertion probability is consistent with the exponential approach of the coverage fraction \theta(t) to the jamming limit \theta_j.

O.S.IV.2.

Inkjet printing of TiO_2 nanoparticles on flexible substrates

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The presented research focuses on development of functional dispersion of TiO_2 nanoparticles in the form of ink, which could be used for the inkjet printing of thin films on various substrates. Arabic gum from acacia tree was used to control the viscosity of the prepared ink and to serve as binder for nanoparticles on the surface of substrate. Particle size distribution measurements with Z-sizer revealed that TiO_2 nanoparticles have uniform distribution centered at around 120 nm. In order to determine the most suitable substrate for printing of the ink, water contact angle measurements were performed on Si, kapton and PET surfaces. The deposition of the ink was carried-out with Dimatix DMP-3000 piezo-controlled inkjet printer. Several layers of nanoparticles were printed on interdigitated electrodes in order to determine the optimal number of layers which will yield best electrical and humidity sensing performance. The characterization of electrical properties of the printed thin films was performed in the DC regime. Printed films were tested as humidity sensor components and obtained results point out to high sensitivity towards humidity with relatively fast response/recovery times.

O.S.IV.3.

Photocatalytic hollow TiO_2 and ZnO nanospheres prepared by atomic layer deposition

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In our research, carbon nanospheres were prepared by hydrothermal synthesis, and coated with TiO_2 and ZnO nanofilms using atomic layer deposition. Subsequently, through burning out the carbon core templates hollow metal oxide nanospheres were obtained. The substrates, the carbon-metal oxide composites and the hollow nanospheres were characterized with TG/DTA-MS, FTIR, Raman, XRD, SEM-EDX, TEM-SAED and their photocatalytic activity was also investigated. The results indicate that carbon nanospheres are not beneficial for photocatalysis, but the crystalline hollow metal oxide nanospheres have considerable photocatalytic activity.

O.S.IV.4.

Preparation of iron tungstate ($FeWO_4$) nanosheets by hydrothermal method

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The influence of sulfate and iron containing additives on the hydrothermal reaction of sodium tungstate (Na_2WO_4) and hydrochloric acid (HCl) was investigated. The products were screened by XRD and SEM. The used additives (Na_2SO_4, $FeSO_4$, $(NH_4)_2Fe(SO_4)_2$, $NH_4Fe(SO_4)_2$, $FeCl_3$) and reaction temperatures (180 and 200 °C) had significant effect on the composition and morphology of the products. Oxalic acid as additional reagent improved the crystallinity in all cases. We prepared 20-30 nm thick and 0.5-1 μm wide $FeWO_4$ nanosheets for the first time using $FeSO_4$ at 200 °C, while 50-300 nm thick and 5-10 μm long h-WO_3 nanorods were obtained with Na_2SO_4 at both temperature. The other additives resulted heterogenous products, containing other phases. $FeWO_4$ nanosheets and h-WO_3 nanorods were analyzed by EDX, TEM, FTIR, Raman, UV-Vis, and their photocatalytic activity was measured. The $FeWO_4$ nanosheets (Ebg = 1.73 eV) were 2.5 times better photocatalysts than h-WO_3 nanorods (Ebg = 3.05 eV).

O.S.IV.5.

Preparation and investigation of the photocatalytic properties of core/shell nanocomposites

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We studied the photocatalytic properties of atomic layer deposition (ALD) grown amorphous and crystalline TiO_2 and as reference, ALD deposited amorphous Al_2O_3 and crystalline ZnO. The oxide layers were deposited on sol-gel SiO_2 and emulsion polymerized PMMA (poly(methyl-methacrylate)) nanoparticles, as well as on electrospun PVA (poly(vinylalcohol)) and PVP (poly(vinylpyrrolidone)) nanofibers. Besides core/shell nanoparticle and nanofiber composites, oxide nanotubes were obtained as well by removing the polymer core by annealing or dissolution. The as-prepared samples were investigated by SEM-EDX, TEM, FT-IR, Raman and XRD. The photocatalytic properties were analyzed by the decomposition of aqueous methylene orange, monitored by UV-Vis. As expected, the Al_2O_3 was not active. The crystalline ZnO and TiO_2 showed good photocatalytic activity. The amorphous TiO_2 had considerably smaller, but still detectable activity. This is a novel result, as previously amorphous TiO_2 was considered to be photocatalytically inactive. ALD grown amorphous TiO_2 is thus unique.

O.S.IV.6.

Reductive properties of nanocrystalline Al-modified cobalt oxides: in situ XRD investigation

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It is known that nanocrystalline Co_3O_4 shows good activity in CO oxidation. Also Co_3O_4 is oxide precursor of metal Co containing supported catalysts of Fischer-Tropsch synthesis. So studies of reductive properties of Co_3O_4-based oxides are very actual. TPR curves usually contain two narrow peaks showing two-step reduction: $Co_3O_4 \rightarrow CoO \rightarrow Co$. Co_3O_4 supported on γ-Al_2O_3 shows another reduction behavior. The complex reduction of the supported catalysts is reported to be due to the chemical interaction of cobalt oxide with the Al_2O_3 support. Generally, the interaction between a metal oxide and a carrier is classified into three categories: (a) very weak interaction in which the support acts only as a dispersing agent, (b) solid solution formation, and (c) strong interaction or surface compound formation. In TPR studies supported not interacted Co_3O_4 particles are reduced at temperatures close to the reduction temperature of bulk Co_3O_4 (550-650K). Stoicheometric spinel $CoAl_2O_4$ formed by solid state reactions between cobalt and the support requires reduction temperatures as high as 1200 K. However, there are many different opinions about phases, which are reduced in the intermediate temperature range 650-1200 K. To clarify this question, the present study was focused on the detailed phase and structural characterization of Co-Al oxide reduction in H_2. Mixed oxides were prepared by coprecipitation of Co^{2+} and Al^{3+} ions at different Al:Co ratios. It was very important to examine the reduction of Al-modified Co_3O_4 in situ, because for this system ex situ investigations may not represent the actual state of the cobalt-containing phase under reduction conditions.

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O.S.IV.7.

Non-destructive testing of cover made of CFRP after ballistic impacts by IR thermography methods

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Multi-layered composites are frequently used in many military applications as constructional materials and light armours protecting personnel and armament against fragments and bullets. One of the many methods used in non-destructive testing of composites is active infrared thermography. In active thermography it is necessary to deliver energy to the examined sample in order to obtain significant temperature differences indicating the presence of subsurface anomalies. To detect possible defects in composite materials different methods of thermal stimulation can be applied to the tested material, these include heating lamps, lasers, eddy currents, microwaves or ultrasounds. The use of a suitable source of thermal stimulation on the test material can have a decisive influence on the detection or failure to detect defects. Non-destructive testing was carried out using the following sources of thermal stimulation, heating lamp, flash lamp, ultrasound and eddy currents. The paper presents the possibility of applying IR thermography methods for detecting defects in ballistic covers made of carbon fiber reinforced composites used in the construction of military vehicles.

O.S.IV.8.

Ductile/brittle polymer system modified with carbon nanoplatelets: Effect of components coupling

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Addition of different nanoparticles may significantly upgrade performance of multicomponent polymer systems. Their effect is more complex in comparison with single-matrix nanocomposites due to combination of reinforcement with marked structure-directing effects, interphase modifications, etc. This work deals with upgrading the ductile/brittle polyamide 6 (PA6)/polystyrene (PS) system with amine-modified carbon nanoplatelets (GNP). Here, the styrene-maleic anhydride copolymer reacts with PA6 and GNP, and its use allows in-situ formation of a GNP-based adduct. The effect of mixing protocols on structure of polymer chains modified with GNP and its impact on the PA/PS system performance are discussed. This includes size of the dispersed PS phase, its plastic deformation during loading, PA6 matrix crystallinity, rheological behaviour and dynamics reflected in influencing of glass transition temperature. Harmonization of these effects allows preparing PA6 material with substantially enhanced well balanced mechanical properties.

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O.S.IV.9.

Neutron and synchrotron diffraction studies of low dimensional frustrated magnets with unique magnetic, electrical and redox properties

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High-resolution neutron and synchrotron diffraction studies of the magnetic structures of $Na_3Co_2SbO_6$, $Li_3Ni_2SbO_6$ and $Na_2Ni_2TeO_6$ layered oxides with a honeycomb superstructure are presented. These compounds are expected to be promising materials as solid electrolytes or electrode materials, thermoelectric materials, superconductors and unusual magnets with low-dimensional magnetic ordering, spin-flop transitions, etc. Their magnetic properties are important because the processes of ionic transfer are connected with the change of the valence and spin states of transition metals. AFM type interaction between nearest, second and third nearest neighbors can lead to frustration in the magnetic subsystem and the emergence of unusual types of magnetic moments ordering including stripe, zigzag and different spirals. Despite an essential difference in the crystal structure, namely in the packing of honeycomb layers along c-axis, magnetic structures for all samples can be considered as zigzag FM chains AFM coupled. However, zigzag type is very different for each compound.

O.S.IV.10.

The study of the correlation between surface chemistry and charge storage properties of graphene oxide

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The carbon materials have a long history of energy-related applications and have witnessed a new rebirth after isolation of graphene. Thanks to a large specific surface area, electrical conductivity and rich surface chemistry the graphene oxide (GO) have attracted considerable attention for application in electrochemical capacitors. To improve comprehension of its surface chemistry and to evaluate the contribution of particular oxygen functional groups in charge storage properties, the GO was reduced in an inert atmosphere (up to 800 °C). The results, obtained by the Fourier transform infrared spectroscopy, X-ray photoelectron spectroscopy, micro-Raman spectrometry, temperature-programmed desorption and cyclic voltammetry methods, provide better understanding of the interdependence of surface, structural and electrochemical properties of graphene oxide.

O.S.IV.11.

Influence of zinc doping on the magnetic properties of cobalt ferrite nanoparticles

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In the present work, cobalt ferrite nanoparticles with different zinc content ($Co_{(1-x)}Zn_xFe_2O_4$; x=0, 0.05, 0.1, 0.3 and 0.5) but with the same particle size distribution and capping agent were prepared by solvothermal synthesis method. The XRD patterns of samples show that all the diffraction maxima correspond to the cubic spinel structure. TEM analysis revealed the presence of sphere-like particles with similar diameter for all the samples (<DTEM>~5nm). The FT-IR analysis confirms the presence of oleic acid on the surface of the nanoparticles. Field dependence of magnetization recorded at 5 K show an hysteretic behavior with increase of coercive field with decrease of zinc content (HC(CoZn_x_0.5)=0.60 T; Hc(CFO)=1.13 T). Temperature dependence of magnetization, recorded by Zero Field Cooled and Field Cooled protocols, indicates that all the samples are superparamagnetic at room temperature. MZFC show a maximum for all the samples, with Tmax decreasing with the increasing of Zn content.

Poster Presentation

P.S.A.1.

Preparation and properties of photocatalyst in TiO_2-ZnO system

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Titania and zinc oxide nanoparticles have known as the most promising photocatalysts under ultraviolet radiation. The combining of TiO_2 and ZnO will improve the properties of photocatalyst due to interfacial interaction, efficient charge separation of photo-activated electrons and holes, as well as to formation of zinc titanates.

The aim of the present work was preparation of nanoparticles in TiO_2-ZnO system with various ratio of components and determination their photocatalysts activity in dependence on powders parameters.

Particulate TiO_2-ZnO composites were prepared by sol-gel method using $Ti(OC_4H_9)_4$, $Zn(CH_3COO)$, $Ti[OCH(CH_3)_2]_4$, trietanolumine or acetic acid. Specific surface area of the prepared samples was in the range of 12.6-56.8 m^2/g and crystallite size in the range of 10-100 nm depending on the ratio of components and calcination temperature. Increase of Zn/Ti molar ratio from 0.1 to 3.3 leads to decrease of ZnO phase and the formation of titanate phases. The highest photocatalytic activity in degradation of MB solution shows sample prepared at Zn/Ti ratio in the range of 1.0-3.3 and calcinated at 600-700 ºC due to high content of $ZnTiO_3$ phase.

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P.S.A.2.

Modified TiO_2 thin films prepared by spray pyrolysis deposition and their photocatalytic activity

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Nowadays TiO_2 nanoparticles are recognized as active photocatalyst for degradation of organic pollutants under UV radiation. However, direct application of the nanoparticles for water treatment is limited because their separation from water is difficult. From this point of view promising is use of fixed onto substrate photocatalyst.

The aim of the research was elaboration active modified TiO_2 thin films and determination their photocatalytical properties.

TiO_2 thin films were obtained by spray pyrolysis equipment HolmarcHO-TH-04 using titanium(IV) isopropoxide (TTIP) as precursor, acetyl acetone as stabilizer and isopropyl alcohol as solvent. Different concentrations of TTIP solutions were prepared and various modifiers were added. The thin films were made on the heated glass substrate using air as carrier gas at 2 bar pressure. After spraying the obtained samples were annealed in air at 500 ºC temperature for several hours.

The structure and morphology of the thin films were characterized by X-ray diffraction and scanning electron microscopy. Photocatalytical activity was measured by degradation of methylene blue dye under UV irradiation.

P.S.A.3.

Nanobanksia - novel hybrid inorganic/organic nanomaterial

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We have developed an efficient method for fabrication of novel hybrid inorganic/organic nanomaterials composed of molybdenum carbide nanowires densely covered with carbon nanofibres by carburisation of $Mo_6S_2I_8$ nanowire bundles in the mixture of argon/ethane. The BET surface area of obtained hybride material is over 150 m^2 g−1. The carbon nanofibres grown perpendicularly to the surface of molybdenum carbide nanowires have lengths around 100 nm and diameters from 10 to 20 nanometres. In addition, we present a simple, very efficient, single-step selfdecoration water dispersed hybride material with different noble metals nanoparticles (gold, platinum, palladium). The reduction of noble metals chloride complexes takes place at room temperature without any additional reducing reagents resulting in a new family of very promising materials, in particular as catalysts. Several different methods, including X-ray diffraction, scanning electron microscopy with wave dispersive analysis, and transmission electron microscopy were used for characterisation of the starting nanowires and the final products. Based on the experimental observations, we also propose the mechanism for the formation of novel hybrid inorganic/organic nanomaterials.

P.S.A.4.

Leaching of trace elements from packaging material into canned meat products

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The interaction between food and metal packaging might be a potential source of trace elements release, which if ingested by humans can cause harmful effects. The present study is undertaken to investigate the leaching of elements from packaging materials into canned meat products under different conditions of storage period and temperature, as well as the various degrees of the can damage. The meat products are packaged in cans made of electrolytic tinplate, produced by the special requirements of the Army of the Republic of Serbia. Cans are protected inside with epoxy-phenolic, aluminum-pigmented varnish. The structure of the varnish is examined by IR spectroscopy and off-line pyrolysis-GC/MS. Method of Scanning Electron Microscopy with Energy Dispersive-X-ray Spectrometry (SEM/EDS) is used to identify cracks in the varnish during induced mechanical damage. This identification is carried out by comparing EDS spectra (elemental analysis) of the inner surface of the cans, obtained before and after the induced damage. The SEM analysis is used for measuring the surface of the induced damages, i.e. the total contact area of the tin coating with the meat product inside the can. The metal concentrations in the canned foods are determined by Inductively Coupled Plasma with Mass Spectrometry (ICP-MS). The concentration of Cr, Mn, Fe, Cu, Zn, As, Se, Cd, Sn, Hg, Pb and Al is determined when the meat products stored at room and elevated temperature (20 and 40 ºC), within their shelf life storage period and longer, as well as in the content of cans without damage and with various degrees of damage. The concentrations of elements obtained under this study were compared with the recommended limits of FAO/WHO Codex Alimentarius Commission and EU maximum permitted levels. It has been shown that the degree of damage to the cans is directly proportional to the degree of migration of some metals in the canned food.

P.S.A.5.

Characterization of pressure-less sintered MgO-Al_2O_3-SiO_2-TeO_2 system

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In this study, sintering of two systems was investigated in parallel, pure cordierite $2MgO:2Al_2O_3:5SiO_2$, and cordierite with addition of 5 mass % TeO_2. Green bodies were prepared from powder mixtures mechanically activated for 0, 10 and 40minutes by uniaxial pressing at 20 MPa followed by cold isostatic pressing (CIP) at 1000 MPa. The pressure-less sintering of these specimens was performed at a temperature of 1350 ^oC for 1 h, with 10 ^oC/min heating rate. Densities over 96 % of theoretical values were obtained for samples activated for 40 minutes. XRD measurements of MAS-40 sintered sample pointed at a mixture that consisted of several phases, majority of cordierite (> 73 %), spinel $MgAl_2O_4$ (> 22 %), $ZrSiO_4$ (2.5 %), and Al_2O_3 (1.8 %), while XRD pattern of MAS-40-TeO_2 contained majority of cordierite (> 72 %), spinel $MgAl_2O_4$ (> 23 %), $ZrSiO_4$ (1.9 %), and Al_2O_3 (1.9 %).

The relative permittivities of the samples were measured in an open test fixture. The results for the real part of the complex relative permittivity of the samples, measured at 200 MHz, are shown in Table I. The loss tangent for all samples was very small, below the resolution of the measurement setup (0.005).

Table I The real part of the complex relative permittivity and the density of the samples.

	MAS-0	MAS-0-TeO_2	MAS-10	MAS-10-TeO_2	MAS-40	MAS-40-TeO_2
ε'_r	5.236	4.964	4.963	4.987	5.542	5.554
ρ (g/cm^3)	2.45	2.21	2.32	2.29	2.60	2.56

There is a strong correlation between the relative permittivity and the density, which agrees with our previous results.

P.S.A.6.

Temperature responsive hydrogels based on ehylene glycol propylene glycol "block" units with VPTT close to human body temperature

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New hydrogels based on different oligo(alkylene glycol) methacrylate (OAGMA) with inverse thermo-response and volume phase transition temperature (VPTT) close to human body temperature were investigated in this work. Synthesis was performed from monomer-solvent mixture by gamma radiation; four different OAGMA (EG6MA, EG6PG3MA, EG3PG6MA and PG5MA) were used. The main focus was made on hydrogels based on EGxPGy pendant chains with different number of ethylene glycol and propylene glycol units in "block" backbone since in the case of POPGMA and POEGMA homopolimers (e.g. hydrogels with pure PG and EG pedant chains) the VPTTs were observed far below and far above the human body temperature, respectively. Characterisation of the hydrogels was performed by swelling, UV-Vis, FTIR, SEM, DSC and in vitro biocompatibility investigations. Due to the possibility to combined VPTT close to human body temperature with good biocompatibility, new hydrogels based on EGPG "block" pedant chains show great potential for biomedical applications.

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P.S.A.7.

Composition of red mud and/or metakaolin-based modified geopolymers

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There is potential use of red mud for synthesis of inorganic polymeric materials through a geopolymerization process as an alternative in the sectors of construction and building materials. By introducing of inorganic and organic modificators of microstructure (calcium hydroxide, bi-functional epoxy resins, or various types of alkoxylanes) during the geopolymer synthesis the enhanced values of ductility and strength can be obtained.

Research was performed on alumosilicate material (red mud and metakaolin) and alkali activator raw mixture with defined quantity of modificator. The best sinthesys conditions were identified. Post-synthesis curing also play important role in obtaining of good-performing geopolymers. Characteristics of geopolymers were defined by measuring of compressive strength, N2-physisorption, as well as by SEM analysis, X-ray diffraction (XRD) and Fourier transform infra-red spectroscopy (FTIR). In addition the lower value of zeta potential was identified as the assisting factor for the specific structure domains formation (within the certain range of pH) accompanied by the high compressive strength.

P.S.A.8.

Fabrication and characterization of Al-5 wt.% Si matrix composites reinforced with various boride particles

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This study reports the effect of different boride particles on the Al-5 wt.% Si matrix composites produced via powder metallurgy methods (mechanical alloying, cold pressing and pressureless sintering). Metal borides (TiB_2, NbB, VB_2) were prepared in our laboratory facilities from metal oxide (TiO_2, Nb_2O_5, V_2O_5), B_2O_3 and Mg containing blends using mechanochemical synthesis and leaching. To obtain hybrid powders, Al-5 wt.% Si and 2 wt.% boride powders were mechanically alloyed (MA'd) for 0, 1, 4 and 8 h in a high-energy ball mill. Powders were compacted using a hydraulic press under uniaxial pressure of 450 MPa and sintered at 570 C for 2 h under Ar gas. MA and reinforcements improved the density/microhardness values and wear resistances of the composites. Al-5 wt.% Si-2 wt.% TiB_2 MA'd for 4 h exhibited the highest microhardness value (199 HV) whereas Al-5 wt.% Si-2 wt.% VB_2 had the lowest wear volume loss value (0.072).

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P.S.A.9.

Combustion synthesis of yttrium aluminum perovskites doped by rare earth ions

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Yttrium aluminum perovskite (YAP) with an orthorhombic structure is one of the three phases in t the binary Y_2O_3-Al_2O_3 system. Doped by trivalent rare earth transitions metal ions YAP is an important material for optical applications. It is not easy to obtain single-phase YAP ceramic due to the local inhomogeneous distribution of Y-Al ions and simultaneous formation of accompanying YAM and YAG phases. Although demanding, manufacturing pure and dense polycrystalline ceramics is essential for materials with high optical properties.

The aim of this work was to obtain high purity and high density YAP polycrystalline ceramic compact using the wet chemical method for powder preparation followed by pressureless densification. The results were compared with specimens prepared by the solid state reaction method. The $YAlO_3$ and $YAlO_3$:RE^{3+} (RE = Eu, Pr, Ce, Lu) powders were prepared by the wet chemical methods: precipitation, Pechini, combustion and other modifications of the sol-gel method). Specimens were then densified at the temperature range of 900-1650ºC. The morphology of powders was examined in the scanning electron microscopy (SEM) and laser diffraction particle size analyzer (PSD) was used for powder particle distribution after synthesis. The phase composition was measured by x-ray diffraction method (XRD). The Results show that powder synthesis method as well as addition of RE ions significantly influenced the purity, particle size distribution and porosity of ceramic bodies.

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P.S.A.10.

Modification of poly(ethylene terephthalate) by blending with polyamide-6 utilizing reactive compatibilization

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The utilization of polymer blends is increasingly important issue in fiber and polymer industry. Poly (ethylene terephthalate) (PET) and polyamide-6 (PA6) are both semicrystalline polymers as major plastic and textile materials. PET is widely used for packaging bottles and polyamide-6(Nylon6) has advantage such as high moisture absorption and toughness. The blend of PET and PA6 has not drawn the attention because of incompatibility of two polymers. In this study, epoxy resin (YD-019K) was investigated as a reactive compatibilizer for the incompatible polymer blends of PET and PA6. The phases separation, thermal, mechanical and rheological properties of blends were analyzed. It was found that PA6 could be well dispersed in PET matrix by cross-linking effect of epoxy. The domain size of PA6 in PET was controlled to submicron size which is considered enough for the practical uses.

P.S.A.11.

Thermal and mechanical properties of poly(ethylene terephthalate) copolymer containing bis(dimethyl-2-hydroxyethyl) tetraoxaspiro undecane

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Many efforts have been attempted to increase the thermal and mechanical properties of poly(ethylene terephthalate) (PET). In this work, we tried to enhance the thermal and mechanical properties of PET by incorporation of bis(dimethyl-2-hydroxyethyl) tetraoxaspiro undecane (BDHTU) as a comonomer. PET copolymers more than 6 mol% of BDHTU was amorphous. The glass transition temperature of copolymers increased continuously with the composition of BDHTU. The glass transition temperature of PET copolymer at loading of 20 mol% BDHTU was 94º, which was 25º higher than that of PET. The thermal degradation temperature of PET copolymers was decreased with the composition of BDHTU. The mechanical properties of PET and PET copolymers will be measured.

P.S.B.1.

The influence of changes in Ca/Y concentration ratio on the spectroscopic properties of europium doped $Ca_9Y(PO_4)_7$ phosphor for white light emitting diodes

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Recently, white light emitting diodes (w-LED) have become a very popular source of light. There are several methods that lead to obtain white LEDs. For instance one uses the device consisting with a single-composition white-emitting phosphor and an UV LED. This method is very appealing because of the great color rendering index and lower production cost. The single-composition phosphor can be achieved by doping the inorganic matrix with the rare-earth ions. The $Ca_9Y(PO_4)_7$ is selected as the compound, due to its good physical and chemical properties. In this study series of $Ca_9Y(PO_4)_7$ doped with 5% of Eu ions and with different [Ca]/[Y] ratio were synthesized using the Pechini method. Due to the presence of two different cations in the studied matrix (Ca^{2+} and Y^{3+}) that are available for europium substitution the synthesis parameters were selected to obtain the incorporation of the europium ions (5% mol) into the calcium sites only. The phase composition analysis and the spectroscopic measurements were carried out before and after reduction of Eu^{3+}. The XRD patterns show that in all cases the obtained materials consist of pure phase of $Ca_9Y(PO_4)_7$. PLE and PL spectra measured before reduction indicate one or two different Eu^{3+} sites dependently on Ca/Y ratio and also for samples obtained after reduction the luminescence of Eu^{2+} depends on the changes of Ca/Y ratio. The observed differences in Eu^{2+} luminescence are discussed taking into account creation of different compensation defects depending on change of Ca/Y ratio.

P.S.B.2.

Spectroscopic properties of Eu^{2+} and Eu^{3+} doped barium potassium phosphate

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Barium potassium phosphate ($Ba_2K(PO_3)_5$) doped with europium belongs to the hosts able to accommodate both Eu^{3+} and Eu^{2+} ions, which make it useful for white light emitting diodes (WLEDs) based on UV chip technology.

In this work effects of pressure and temperature on the luminescence of Eu^{2+} and Eu^{3+}-doped $Ba_2K(PO_3)_5$ are presented. The luminescence spectra and luminescence decays were measured as a function of temperature and pressure. Depending on the excitation wavelength phosphor shows different luminescence spectra. The emission color was bluish green, when only Eu^{2+} was excited, reddish orange when only Eu^{3+} was excited or white over simultaneous excitation of both ions. At room temperature under excitation with near UV light, the luminescence spectrum consists of broad emission band peaking at 480 nm due to the 4f65d1→4f7 (8S7/2) transitions of Eu^{2+} and several sharp lines between 580 and 710 nm region, ascribed to the 5D0 → 7FJ (J = 0, 1, 2, 3 and 4) transitions in Eu^{3+}. At low temperatures, we observed three different bands related to the 4f65d1 →4f7 transitions in different Eu sites (at 415 nm (A), 450 nm (B) and 505 nm (C)): two Eu sites substituting for Ba^{2+} and one Eu site substituting for K^+.

Under fixed excitation wavelength the effect of increasing of the intensity of Eu^{2+} emission with respect to Eu^{3+} emission was observed for temperature range 5 – 100 K. The nonradiative intersystem crossing was responsible for decreasing of the relative intensity of the Eu^{2+} luminescence for temperature range 150 – 500 K and causes decreasing of the Eu^{2+} to Eu^{3+} luminescence intensity ratio for temperature higher than 150 K. Luminescence decays were measured for selected temperatures and pressures. At 10 K the decays of Eu^{3+} luminescence were single–exponential, with time constant being 3.6 ms. When temperature increases all emissions decay faster and become multiexponential. Decay times slightly decreased with increasing pressure. In the range of 10 – 400 K the decays of 4f65d→4f7 emission in the Eu^{2+} were single–exponential, with time constant being 0.65 μs, 0.62 μs and 0.35 μs for A, B and C emission bands, respectively, and did not depend on temperature. At higher temperatures (from 400 K to 500 K) the luminescence decays become shorter and non–exponential, as the result of thermal quenching. When pressure increases all emissions decay faster.

P.S.B.3.

Effect of external influences on Fe- Cr - based alloys studied by positron annihilation spectroscopy

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The presented paper gives an overview of STUBA activities in the area of investigation of effect of external influences (corrosion, neutron irradiation and He ions implantation) on the properties of Fe-Cr-based alloys by Positron Annihilation Spectrometry.

Via differences in Positron annihilation spectroscopy parameters, the changes due to differences in chemical composition, defects type and its accumulation as well as annealing effectiveness can be clearly evaluated.

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P.S.B.4.

The optimization of EVA monolith synthesis for effective immobilization of Candida rugosa lipase

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Among the great variety of enzymes, lipases are most widely used in synthetic organic chemistry as well as industry. In order to exploit their outstanding properties, great attention has been paid to development of ideal solid support for enzyme immobilization. In this work lipase from Candida rugosa has been attached on monolith material based on methacryloyl modified ethylene vinyl acetate copolymer (EVA), glycidyl methacrylate (GMA) and ethylene glycol dimethacrylate (EGDMA). Characterization of modified EVA copolymer, monolith before and after enzyme immobilization was conducted by FTIR and Raman analysis, and wetting angle determination. The immobilization of the enzyme was carried out by two techniques: adsorption and covalent linking. Comparison of the results of activity recovery after immobilization, using both techniques, showed that covalent bonding proceeds through a multipoint covalent attachment and provide more effective immobilization compared to the adsorption technique. After complete immobilization of the enzyme 63% of its initial activity was retained.

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P.S.B.5.

Transport properties of Ar^+ in Ar/CF_4 mixtures for technological applications

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In this work we present a cross section set for Ar^+ in Ar/ CF_4 mixtures where existing experimentally obtained data are selected and extrapolated. Monte Carlo simulation method is applied to accurately calculate transport parameters in hydrodynamic regime. These data are needed for modeling in numerous applications of technologically important. We discuss new data for Ar^+ ions in Ar/ CF_4 mixtures where mean and characteristic energy, flux and bulk values of reduced mobility are given as a function of reduced electric field E/N (E-electric field, N-gas density). We find that internally resonant exothermic dissociative charge transfer cross section for CF^{3+} production significantly increases zero field ion mobility with respect to the polarization limit.

P.S.B.6.

Optimization of magnetoimpedance sensing properties of FeCuNbSiB amorphous microwires

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In this paper magnetoimpedance (MI) effect of $Fe_{73}Cu_1Nb_3Si_{13.5}B_{9.5}$ alloy microwires for magnetic sensor application has been investigated. Amorphous wires with 150 μm of diameter d were produced from arc-melted ingot of master prealloy by in-rotating water spinning technique. The MI measurements were performed in the longitudinal direction of samples by four-point method using LCR HiTester in a dc axial magnetic field Hex produced by 1D-Helmholtz coils. MI ratio of microwires defined as DZ / Z = [Z(Hex) - Z(Hmax)] / Z(Hmax) was explored in amorphous/as – cast state up to the maximum value of the magnetic field Hmax = 17.5 kA/m. MI – effect was studied as a function of external magnetic field Hex, driving frequency f as well as sinusoidal ac current amplitude Iw.

Correlations between in – phase R and reactive X components of impedance Z with electromagnetic skin effect i.e. penetration depth δm were performed, with aim to optimize MI – element sensitivity. Critical frequency of about 30 kHz (when δm ≈ d/2) was observed as the point with the initial increase of the MI. Maximum observed MI – ratio is 26 % at a frequency of f = 1.2 MHz, external magnetic field of Hmax = 17 kA/m and current amplitude Iw = 10 mA. The influence of the sinusoidal ac current amplitude Iw on the penetration depth dm is over bamboo-like magnetic domains structure. As a conclusion, amorphous (micro) wires can be successfully applied for MI based sensors in the high – frequency range (~MHz). Possible applications of this magnetic sensor were discussed.

P.S.B.7.

Improvement of cup anemometer class by bearing design

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Invented in year 1846, the cup anemometer is still a standard instrument for wind potential assessment. The International Electrotechnical Commission (IEC) Standard 62400-12-1 exclusively prescribes the use of cup anemometers for simultaneous measurement of wind speed and power output of a given HAWT at test side. New, more sophisticated techniques for remote sensing of wind speed, like LIDAR and SODAR, were tested using cup anemometer as a reference. The cup anemometer acts as a vertical axis wind turbine which generates output signal proportional to the wind speed. It is a robust instrument which combines simplicity and accuracy and is also used for energy production forecast and wind turbine control during a wind farm operation. In long-term operation, cup anemometers require recalibration, rotation speed is changed due to bearing friction wear, vibration phenomenon due to so called dry friction whip was detected as well as staling effect of heavy snow. These drawbacks shall be assessed or minimized by the improvement of the design. Design improvement includes rotor aerodynamics, shaft-bearing tribology and output signal conditioning. This paper deals with the internal rotating parts tribology. Cup anemometers are classified by the class number k and the class types A and B where class A covers flat and class B complex terrain flow conditions. A class number 1 corresponds to 1% uncertainty at 10 m/s but more than 1% below 10 m/s and less than 1% above 10 m/s. The alphanumeric indices qualify a sensor as class 1. A cup anemometer contains rotating bearings of plain or ball type. Ball bearings prevent sliding friction, lower the friction torque and are more suitable for long-term operation. RNRG class 1 and #40C anemometers have the same form factor and similar inclined flow performance characteristics. The only difference in design is that class 1 anemometer uses ball bearings instead of #40C beryllium copper shaft and bearing made of self-lubricated modified Teflon. Class 1 anemometer is evaluated as class 1.01A and class 8.4B, while #40C as class 2.4A and 7.7B. The flow inclination angle affects both aerodynamic and friction torque. We applied so called Angular Speed Decrement model to calculate the relative contribution of friction and aerodynamic effects to transfer function offset of RNRG class 1 and #40C anemometers. Based on calibration curves, the RNRG #40C calculated offset due to friction was 0.1637 m/s and that of RNRG class 1 anemometer 0.0756 m/s. The analysis of long-term in pair operation of RNRG class 1 and #40C anemometers provided quantification evidence that sensors are interchangeable for wind sensors application, but compared to #40C, class 1 anemometer did not show the degradation (David F. Matson and Gregory S. Poulis in AWEA Wind power 2015). We analyzed the design of several type anemometers. This analysis shows that the exchange of plain bearings by the ball bearings improves the anemometer class and long-term operation characteristics.

P.S.B.8.

Determination of the elastic modulus of partially intercalated and exfoliated polymer-clay nanocomposites using numerical homogenization techniques

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The main purpose of this work is to study the elastic properties of a polymer/clay nanocomposite. The elastic modulus of partially intercalated and exfoliated polymer-clay nanocomposites have been studied using numerical homogenization techniques based on the finite element method. The representative volume element was employed here to capture nanocomposites microstructure, where both intercalated exfoliated and clay platelets coexisted together. The effective macroscopic properties of the studied microstructure are obtained with two boundary conditions: periodic boundary conditions (PBC) and kinematic uniform boundary conditions (KUBC). The effect of particle volume fractions, aspect ratio, number and distribution of particles and the type of boundary conditions are numerically studied for different configurations.

This study presents also the performance of several classical analytical models as Mori and Tanaka model, Halpin and Tsai model, generalized self consistent model through their ability to estimate the mechanical properties of nanocomposites. A comparison between simulation results of polypropylene clay nanocomposites, analytical methods and experimental data has confirmed the validity of the set obtained results.

P.S.B.9.

Production of 99Mo/99mTc generators - Advantages of dry column

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Due to its favorable nuclear properties Tc-99m is the most used radioisotope in nuclear medicine. The main source of Tc-99m is 99Mo/99Tc generator based on (n,f)99Mo adsorbed on alumina. These types of generators are designed to operate either in the “wet” or “dry” mode. A reservoir of saline, in “wet” generator, sufficient for all elutions during the whole life time of the generator, is usually housed in the bottom of the same generator. After each elution, in column remains small amount of saline, which can lead to the occurrence of free radicals in eluate. “Dry” mode presumes that after each elution the rest of saline is removed by passing air through the column which reduces the possibility of occurrence of free radicals in eluate. Numerous studies show that 99mTc from “dry” generator gives better stability of labeled products. This type of generator has been developed in the Laboratory for Radioisotopes (Vinča Institute of Nuclear Sciences, University of Belgrade) and its routine production lasts now already over 35 years.

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P.S.B.10.

High-energy spectroscopy of YbM_2P_2 compounds

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We have studied experimentally and theoretically the electronic structure and x-ray absorption spectrum at the Yb L3 -edge and x-ray emission spectra of M and P at the K- and L2,3 -edges in the mixed valence compound YbM2P2 (with $ThCr_2Si_2$ type crystal structure), where M=Fe, Co, Ni. The theoretical calculations have been carried out by means of the ab initio fully-relativistic spin-polarized Dirac linear muffin-tin orbital method. The calculations show good agreement with the experimental measurements. The LSDA +U with Ueff > 8.8 eV produces two independent self-consistent solutions $YbNi_2P_2$ with divalent Yb^{2+} and trivalent Yb^{3+} ions. For the divalent Yb ion we found a non-magnetic solution with fourteen 4f electron bands completely occupied and situated far below the Fermi level. For trivalent Yb^{3+} solution thirteen 4f electron bands are situated well below the Fermi level. The hole 4f level for the Yb^{3+} solution the completely empty and situated sufficiently far from the Fermi level, therefore $YbNi_2P_2$ belong to the in homogeneously mixed-valence compounds. The calculated total magnetic moment for the Yb^{3+} solution moment is dominated by the 4f compounds, the spin Ms and orbital Ml moments are 0.365 μB, and 1.135 μB, respectively. The spin and orbital moments at the Ni and P sites are very small: Ms Ni= - 0.0028 B, MsP=-0.0017 μB, MlNi =-0.0019 μB and MlP =0.0004 μB. Both the trivalent and the divalent Yb ions in are reflected in the experimentally measured Yb L3 x-ray absorption spectrum simultaneously. We found that the best agreement between the experimental spectrum and sum of the theoretically calculated Yb^{2+} and Yb^{3+} spectra is achieved with 73% ytterbium ions $^{2+}$ state and 27% ions in $^{3+}$ state. We found that the effect of the electronic quadrupole E2 transitions as well as the core-hole effect in the final states has minor influence on the intensity and the shape of the Ni and P K and L2.3 emission spectra as well as on the Yb L3 absorption spectrum. We would like to point out that the LSDA +U method which combines LSDA with a basically static, i.e. Hartree-Fock-like, mean –field approximation for a multi-band Anderson lattice model does not contain true many body physics. However, this method can be considered as the first step towards a better description of strongly correlated electron systems. The LSDA +U method provides the correct energy position of 4f energy bands and gives a reasonable description of the XAS and XES properties in $YbNi_2P_2$. However, the energy band structure for finite temperatures and the presumed Kondo lattice and mixed valence behavior in $YbNi_2P_2$ clearly requires a treatment that goes beyond a static mean-field approximation and includes dynamical effects, e.g., the frequency dependence of the sell-energy.

P.S.B.11.

Influence of electrode thickness on the electrochemical properties of activated ion-track carbon supercapacitors

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We have developed a method for synthesizing flexible thin film supercapacitor electrodes by carbonizing and activating ion-track Kapton foil. The optimization of supercapacitor electrode performance using ion-track technology can be achieved by varying fluence, type, energy and orientation of the ions, as well as varying the thickness of the starting polymer foil and a set of chemical etching conditions. Amongst all of these parameters this paper focuses on analyzing the influence of electrode thickness on electrochemical properties of supercapacitor electrodes, while other parameters will be kept constant. Three thicknesses of starting polyimide film are used 25, 50, 75 µm, all irradiated with Au ions with a fluence of 106 ions/cm^2. The influence of the electrode thickness on the electrochemical properties of the supercapacitor electrodes was investigated by cyclic voltammetry, constant current charge and discharge technique and electrochemical impedance spectroscopy.

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P.S.B.12.

Temperature dependence of relaxation times of quasiparticles in graphene

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The temperature dependence of relaxation times of quasiparticles (electrons and phonons) is analyzed in graphene from the first principles. In the transport processes the various mechanisms of relaxations are essential (electron and phonon scatterings on impurities, phonons, vacancies...). Therefore, relaxation times are found for several characteristic and mostly involved scattering mechanisms of quasiparticles in graphene. This is of fundamental importance for any method applied in further studying of the transport characteristics (solving Boltzmann's equation, using Green's functions...). In particular, the role of relaxation times is important in finding temperature dependence of the coefficients of electronic and thermal conductivities in graphene, as measurable macroscopic transport properties.

P.S.B.13.

Crystal structure and magnetic properties of $Bi_{1-x}Ae_xFe_{1-x}Ti_xO_3$ (Ae=Ca, Sr, Ba) multiferroics

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Inspired by the potential applications of the magnetoelectric effect, interest in multiferroic materials is growing steadily. While $BiFeO_3$ is the most thoroughly studied magnetic ferroelectric compound, the properties of its solid solutions remain a matter of intensive debate. In this paper we show how variation in the chemical composition of $Bi_{1-x}Ae_xFe_{1-x}Ti_xO_3$ (Ae= Ca, Sr, Ba) perovskites affects their crystal structure and magnetic behavior. In particular, our research demonstrates that Ca/Ti and Sr/Ti substitutions suppress the cycloidal antiferromagnetic structure specific to the parent compound, thus stabilizing a weak ferromagnetic ferroelectric state. The Ba/Ti-doped solid solutions retain the magnetic behavior characteristic of the pure $BiFeO_3$. Since the latter observation is directly opposed to the prevailing concept used in describing magnetic phenomena in the $Bi_{1-x}Ba_xFe_{1-x}Ti_xO_3$ series, the origin of the contradiction between the current and previously reported data is analyzed. Finally, the reasons underlying the difference in the magnetic properties of the $Bi_{1-x}Ae_xFe_{1-x}Ti_xO_3$ compounds are discussed.

P.S.B.14.

The fabrication of tubular spinel cobalt manganese oxide by single-spinneret electrospinning as a high-performance electrode for aqueous supercapacitors

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Spinel transition mixed metal oxides (STMMOs) are a class of functional materials with many promising applications in different fields, including electrode materials for supercapacitors. The facile fabrication of spinel cobalt manganese oxide with tubular structure by using two-step process is proposed. This process involves electrospinning of polymers and metal precursors with subsequent calcination in air. The structure and morphology of samples heat-treated at 600 °C for 1, 2 and 3 h has been studied with scanning electron microscope (SEM), while the detection of surface functional groups is performed by Fourier transform infrared spectroscopy (FTIR). The capacitive behavior is investigated in neutral aqueous electrolyte (1M Na_2SO_4) by using cyclic voltammetry (CV), and electrochemical impedance spectroscopy (EIS). As a result, the spinel $CoMn_2O_4$ exhibited the highest specific capacitance of 180 F g^{-1} at a sweep rate of 100 mV s^{-1} in 1M Na_2SO_4 which shows promise for application in supercapacitors.

P.S.C.1.

Effect of W-doped TiO_2 nanopowders on photocatalytic degradation of selected psychoactive drugs

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Amitriptyline and alprazolam are representatives of a large group of psychoactive drugs, where amitriptyline is used for treating depression, anxiety, and chronic pain syndromes, while alprazolam possesses anxiolytic, sedative and hypnotic properties. These drugs are continuously introduced into the environment and consequently more attention is paid to find efficient method for their removal. Efficiency of W-doped TiO_2 nanopowders in photodegradation of alprazolam and amitriptyline was investigated under simulated solar irradiation (SSI). All nanopowders have shown higher efficiency in the photodegradation of amitriptyline in comparison to TiO_2 Degussa P25. Among them TiO_2 doped with 0.4 mol% of W(VI) has shown the highest efficiency. The effects of substrate type, catalyst loading, and initial substrate concentration on the efficiency of photocatalytic degradation using SSI were examined. Besides, the identification of the reactive species and their role in the photocatalytic degradation of amitriptyline and alprazolam under SSI was carried out by using various scavengers.

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P.S.C.2.

Activity of pure ZnO and ZnO/MWCNTs nanoparticles in degradation of clomazone under different type of irradiation

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With rapid development of worldwide industry, increasing environmental pollution has become one of the biggest challenges of our society. Photocatalysts offer great potential for converting photon energy into chemical energy and therefore decomposing organic contaminants. The aim of this work was to investigate removal of the pesticide clomazone from double distilled water in the presence of pure ZnO nanoparticles and ZnO/multi-walled carbon nanotubes (MWCNTs) under UVA and simulated sunlight. The ZnO photocatalysts were synthesized by precipitation method from the water and ethanol solutions of the corresponding metal precursor, while the preparation of the MWCNTs nanocomposites has followed the similar procedure with the addition of pristine nanotubes. Degradation of the pesticide was monitored by UFLC–PDA technique and mineralization was studied by ion chromatography measurements. The performances of the applied photocatalysts were correlated with their physico-chemical properties. Additionally, the activity of commercial photocatalyst and novel nanocomposites under simulated sunlight was compared.

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P.S.C.3.

In-situ study of the oxygen-induced transformation of pyrochlore $Ce_2Zr_2O_{7+x}$ to the kK-$Ce_2Zr_2O_8$ phase

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The temporary storage of oxygen in a solid catalyst is imperative for many important industrial oxidation reactions in the gas phase, for instance the HCl oxidation reaction (Deacon process) and the post-treatment of automotive exhaust gas. A peculiar mixed Ce-Zr (1:1) oxide, the so-called kK-$Ce_2Zr_2O_8$ phase, is a promising material exhibiting an extraordinarily high oxygen storage capacity (OSC) and high stability. We elucidated the temperature-dependent reversible transformation between the pyrochlore pyr-$Ce_2Zr_2O_7$ and kK-$Ce_2Zr_2O_8$ phase upon oxygen uptake and release by X-ray diffraction, X-ray absorption and Raman spectroscopy under in-situ conditions, providing invaluable insights into the structural changes on the atomic level, which are at the heart of the extraordinarily high OSC.

P.S.C.4.

One-step production of nanoalloys in Pt-Co, Pt-Fe, Pt-Ni systems

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In this paper we present results on the synthesis of equiatomic nanoalloys in Pt-Co, Pt-Fe, Pt-Ni systems by thermolysis of precursor compounds. As such, oxalate-metalates of ammines of platinum(II) are chosen. Oxalate-ion and ammonia as ligands allow thermal destruction of the initial complex compounds at low temperatures (250-500 degree of Celsius) to form a pure metallic phase, the ratio of metals in which is strictly specified by the stoichiometry of the parent precursor compound. Varying the conditions of thermolysis (temperature, heating rate, aging time, etc.) makes it possible to produce a variety of products: thermodynamically stable or metastable alloys. The change of the atmosphere of thermal destruction allows obtaining both metallic solid solutions and mixed oxide phases. Varying the temperature of the end of the thermal process and the annealing time makes it possible to vary the size of the nanoalloys, which is very important for further use in catalysis.

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P.S.C.5.

Liquid phase sodium intercalation into layered transition metal chalcogenides

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Transition metal chalcogenides (TMC) attract attention of many scientists due to their semiconducting, optoelectronic properties and as energy storage materials. Ability of layered transition metal calcogenides (MoS_2, WS_2, NbS_3, $NbSe_3$ etc.) to intercalate lithium atoms was presented over the last decades. Lithium, however, is a relatively expensive material because its natural sources are limited. Sodium, due to its similar ionic size and cheapness can be used instead of lithium. In this work we used reaction of transition metal chalcogenides with sodium naphthalenide ($NaC_{10}H_8$) as model process which yields sodium TMC intercalation compounds. Obtained substances were characterized by powder x-ray diffraction, Raman scattering technique, and other methods. Compositions of obtained compounds were also determined.

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P.S.C.6.

Temperature dependence of morphology and size of ZrS_3 and TiS_3 particles in colloidal dispersions

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Transition metal trichalcogenides MQ_3 (M =Ti, Zr, Hf, Nb, Ta; Q = S, Se, Te) are promising materials for electrics, photocatalysis, energy storage due to their unusual electrical and optical properties. These compounds have quasi-one dimensional structure: triangular prisms of chalcogen atoms with metal atom in the center of each prism are arranged in parallel chains. Chains form layers held together by van der Waals forces. Thus, additionally MQ_3 structure is layered, so bulk trichalcogenides can be exfoliated down to nanosized particles. Previously we prepared ZrS_3 and TiS_3 colloidal dispersions via ultrasonication in organic media. In this work we have shown how morphology and size of ZrS_3 and TiS_3 particles in sols depend on temperature of bulk trisulfides synthesis.

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P.S.C.7.

Oxidative longitudinal unzipping of short MWCNTs toward graphene nanoribbons

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Graphene represents unique form of carbon nanomaterials and has enjoyed significant attention due to its exceptional physical and chemical properties. The bulk quantities and solution processability of graphene materials are challenges that are yet to be addressed in order to employ these materials more intensively for industrial purposes. We have demonstrated an effective and facile solution-based method for transformation of short MWCNTs to graphene nanoribbons (GNRs). The synthesis of GNRs was preceded by the cutting procedure of the original long MWCNTs by means of the combined Ag-catalyzed oxidation reaction and ball milling procedure. After the cutting, the obtained short MWCNTs were treated in the acidic medium, followed by their oxidative longitudinal unzipping to form GNRs. Multiple characterization techniques, including X-ray diffraction, transmission electron microscopy, Raman spectroscopy, Fourier transform infrared spectroscopy, as well as the thermogravimetric analysis were used for structural and morphological characterization of as-synthesized GNRs.

P.S.C.8.

Selectivity manipulation of ultrathin film-structure optical characteristics

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Based on innovated theory of optical processes in multilayered ultrathin molecular crystalline films, the optical characteristics (refraction, 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 reflections, scatterings, absorptions and transparencies in every layer of that crystalline nanostructure. The four-layered dielectric nanofilms with different but optimized boundary conditions on surfaces were analyzed and some discrete resonant absorption, reflection and transparent peaks were obtained. Their number, position and distribution depend on the five 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 or their coatings/shells construction for drug carrier/delivery in nanomedicine.

P.S.C.9.

Accelerated service life test of electrodeposited NiSn coatings as bifunctional hydrogen and oxygen evolution catalysts for alkaline water electrolysis

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Electrodeposited NiSn alloy coatings were tested for application as cathodes and anodes in the cell for alkaline water electrolysis in 30 wt.% KOH at 80 ºC. The "accelerated service life test" (ASLT) was performed for HER and OER reactions, and compared to those for Ni electrode. The morphology and chemical compositions of the NiSn and Ni coatings were investigated by SEM and EDS, while their surface composition was investigated by XPS before and after the ASLT for both reactions, respectively. It was shown that the cell voltage at $j = 0.3$ A cm^{-2} saving with the NiSn electrodes amounts to about 435 mV before and about 304 mV after the ASLT. SEM results showed that no changes in the morphology of as prepared samples could be detected after the ASLTs for both reactions. EDS and XPS analysis confirmed that some changes occurred during the ASLT, particularly for the oxygen content in the surface layer.

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P.S.C.10.

Zero-dimensional hexagonal stanene nanostructures in magnetic field

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Stanene, low-buckled honeycomb monolayer of tin atoms has been recently synthetized via molecular beam epitaxy. First-principles calculations predicted that stanene is quantum spin Hall insulator, which is a consequence of intrinsic spin-orbit coupling. Stanene has the largest nontrivial bandgap of all group IV monolayers, thus it is the most promising candidate for novel applications considering the quantum spin Hall effect. In this paper, by means of a comprehensive model we explore the bulk-edge correspondence in (quasi) zero-dimensional structures with closed edges subjected to perpendicular magnetic field. The hexagonal flakes and nanorings with zigzag and armchair edges are analyzed. In both of them helical edge states circulating around the outer and inner edges are found. The edge states are found to have properties strongly dependent on the structure geometry and are affected by the edge type.

P.S.C.11.

Three novel bis-phosphonate-coated MNPs labeled with 99mTc as multifunctional agents for possible use in medicine

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The multifunctional nanoparticles, based on magnetite nanocore, are modified with three hydrophilic and biocompatible bis-phosphonate ligands: 2,3-dicarboxypropane-1,1-diphosphonic acid (DPD), hydroxymethylene diphosphonate (HEDP) and methylene diphosphonate (MDP). Characterization of MNPs was performed using X-ray powder diffraction, transmission electron microscopy, Fourier transform infrared spectroscopy, dynamic light scattering and zeta potential measurement. The heating ability for cancer hyperthermia therapy application was quantified through the specific power absorption (SPA) measurement and found to be 76, 131, 186 W/g for Fe_3O_4-DPD, Fe_3O_4-HEDP and Fe_3O_4-MDP, respectively. Conditions of labeling with 99mTc, such as pH, concentrations of MNPs, Sn(II):MNPs mole ratios and reaction time were varied to obtain maximum radiolabeling yield. Bis-phosphonate-coated MNPs were 99mTc-labeled in reproducible high yields (>93 %). All presented positive attributes make these MNPs possible theranostic agents with potential capability to perform concurrent tracking, imaging and therapeutic application.

The authors acknowledge the financial support from the FP7-ERAChairs-MAGBIOVIN—project and the Serbian Ministry of Education, Science and Technological Development (Grant No. III45015).

P.S.C.12.

Spectral analysis of the ordering effect of starch coated magnetite nano-particles

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The aim of this work was to investigate changes of the optical transmittance of the ferrofluid suspension in a magnetic field. Magnetite nanoparticles coated with starch have been synthesized using a coprecipitation method. The effects of magnetic field on magnetic particles in suspension were examined in detail. That was tracked by white-light and laser irradiation of the sample and measuring a transparence of ferrofluid suspension. We have paid special attention on the spectral region in which the greatest changes of intensity of transmitted light corresponds to the wavelength range of 650-670 nm. In this spectral region a lot of monochromatic sources of coherent radiation are developed, and often used for therapeutic purposes.

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P.S.C.13.

Electrospun PMMA nanofibers doped with CdSe/ZnS core shell quantum dots

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This paper presents processing and characterization of composite nanofibers poly (methyl methacrylate)- CdSe/ZnS core shell quantum dots (QD). Nanofibers of pure PMMA and composites with 0.06 % wt. CdSe/ZnS core shell quantum dots nanoparticles were made using electrospinning method. Characterization of starting components and composites was performed in order to obtain information of their morphology, structure, thermal stability, mechanical and optical properties. DSC analysis has shown an increase in Tg for composite with QD. Optical studies by time resolved laser induced fluorescence (TR-LIF) showed that the size-tunable optical properties can be achieved in the polymer nanofibers by addition of quantum dots.

P.S.C.14.

Formation of nanocrystalline 9R silicon hexagonal phase under multi-ion implantation into Si and SiO_2/Si substrates

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The silicon and thermally oxidized silicon substrates were multi-ion implanted by Ga^+ (80 keV), N^{2+} (40 keV) with subsequent annealing at 800 °C (30 min). Some samples were preliminary subjected to N^{2+} (20 keV) implantation with postannealing at 1100 °C. The formation of nanocrystalline 9R hexagonal phase was revealed by cross-sectional electron microscopy. The nanocrystals are located below the ion-amorphized layer in bare silicon substrate and below the oxide film in the SiO_2/Si substrate. The mechanism of 9R phase formation is proposed to be associated with the relaxation of stress induced by ion implantation.

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P.S.C.15.

Enhancing Pt catalytic properties by addition of Au: Could less be more?

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PtAu/C nanocatalysts have been successfully used in electrooxidation of formic acid, due to their good electrocatalytic properties for this reaction - good activity and stability due to high CO poisoning resistivity. The result of such composition of the catalyst is that formic acid electrooxidation proceeds preferably through a direct mechanism pathway, which does not involve CO formation as a reaction intermediate. In the previous studies, it was shown that the convenient catalyst atomic composition for such effect is at least 4 times more Au than Pt. However, the aim of this study is to show that the same effect can be observed even on low loading catalysts with much smaller portions of Au, provided their proper distribution on the surface of Pt nanoparticles.

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P.S.C.16.

Texture evolution of Cu single crystals after drawing

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The main aim of present work was to reveal the differences in microstructure and texture formation two copper single crystals <111> and <110> after drawing process. For detailed microstructure investigations, a Transmission Electron Microscope (TEM) was used. The observations of deformed microstructures were performed on the JEOL 1200 transmission electron microscope with an accelerating voltage of 120 kV. The TEM samples were mechanically ground to ~ 20 µm thickness followed by twin-jet electropolishing at 20 V DC. Grain size was determined by calculating the equivalent diameter (d_2), which means the diameter of a circle with an area equal to the investigated grain. 200 randomly selected grains were determined for grain parameter calculation. The global texture measurements after deformation were performed using a Bruker D8 X-ray diffractometer set up with Kα radiation filter for Co anode. The measurements were recorded within a 5°x5° mesh and a beam intensity at 5 second intervals.

The revealed study showed the differences in the quantitative results of the texture as well as significant differences in the formed microstructure.

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P.S.D.1.

Magnetite functionalized cellulose membranes for heavy metal removal from water

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Magnetite (MG) functionalized cellulose membranes with different pore diameter (10 μm and 0.9 μm) were used as adsorbent for heavy metal (cadmium and nickel) removal from natural water. Controllable precipitation of MG from solvent/nonsolvent system was performed on chemically modified cellulose membranes with 3-(carbomethoxy)propionyl chloride (CPC), in the first step, and with branched polyethylene imine (PEI), in the second step. The effectiveness of cellulose membranes modification was confirmed applying FTIR, Raman and XRD analysis. Comparative adsorption study, related to benefits of pore diameter size, i.e. 10 μm versus 0.9 μm, for the MG functionalized cellulose membranes for lead and nickel removal was conducted. In a batch test, the influence of cellulose membranes mass and contact time on adsorption efficiency of Cd^{+2} and Ni^{+2} ions were studied. High adsorption capacities, 51.7 mg g^{-1} and 54.4 mg g^{-1} for Cd^{+2} and Ni^{+2} ions, respectively, were obtained using MG functionalized cellulose membranes with pore diameter of 0.9 μm, while lower capacity (28.8 mg g^{-1} and 40.9 mg g^{-1} for Cd^{+2} and Ni^{+2} ions, respectively) were obtained using MG functionalized cellulose membranes with pore diameter of 0.9 μm.

P.S.D.2.

Application of NIR spectroscopy in study of adsorption process of p-nitrophenol on activated carbon in presence of selected amides

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This study is a spectroscopic contribution to better understanding of adsorption behavior of some water pollutants in solid/liquid interfaces. We report application of NIR spectroscopy in treatment of water polluted with aromatic organic compounds, such as p-nitrophenol, in presence of amides as products of possible decaying biomaterial. Kinetic of adsorption process of p-nitrophenol on activated carbon was followed by aquaphotomic method. Namely, by measuring the absorption of first overtone of water in NIR range, we were able to gather some valuable information about mechanism of adsorption process, and to follow structural changes in solutions caused by drop in concentration of solutes.

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P.S.D.3.

Calorimetric research of arsenate adsorption on silica-based materials

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Adsorbent based on macroporous silica, impregnated with hydrous iron oxide (goethite), was synthesized in two-step process. The first step included introduction of amino active sites by silica surface modification with (3-aminopropyl)trimethoxysilane, while the second step included concentration of $FeSO_4x7H_2O$ and $FeCl_2x4H_2O$ on the surface of the amino modified silica. Iron oxide was precipitated in goethite form by ferri/ferro oxidation, performed in air, and following by neutralization with $NaHCO_3$ buffer solution. Different diameters of finally produced particles were obtained, up to 1 mm. Arsenate ions were adsorbed from aqueous solutions (~ 0.002 M); the adsorption was studied by measuring the adsorption heats using differential heat flow calorimeter (TITRYS from Setaram) equipped with a stirring system and a system for the introduction of liquids. The amounts of adsorbed pollutant were obtained in separate sets of experiments. The adsorbents show the adsorption capacities comparable with the other solids used for the same purpose.

P.S.E.1.

Mono- and dinuclear azido Co(II) complexes with the condensation product of 2-quinolinecarboxaldehyde and Girard's T reagent

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Mono- (1) and dinuclear (2) azido complexes of Co(II) with the condensation derivative of 2-quinolinecarboxaldehyde and Girard's T reagent (HLCl) were synthesized in the reaction of the ligand HLCl, $Co(BF_4)_2 \cdot 6H_2O$ and NaN_3. Complexes 1 and 2 were characterized by elemental analysis, IR spectroscopy and X-ray crystallography. In both of the complexes hydrazone ligand is coordinated through the quinoline nitrogen, the imine nitrogen and the carbonyl oxygen atoms. Octahedral environment in mononuclear Co(II) complex (1) consist of one molecule of tridentate HL ligand and azide monodentates at the rest of coordination places. In dinuclear double end-on azide bridged Co(II) complex (2) octahedral surrounding around each of two Co(II) centers consist of NNO coordinated deprotonated hydrazone ligand, one monodentate azido ligand and two azido bridging ligands. Due to their interesting structural properties complexes 1 and 2 can be of interest as biologically active compounds.

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P.S.E.2.

Calvarial defects in rats filled with innovative nanocomposite material. Histological and biochemical studies

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Healing of calvarial defects in rats was performed with nano composite material of chitosan/nano hydroxyapatite composite. Nano hydroxyapatite powder was synthesized using 3 steps method: (1) precipitation from $Ca(NO_3)_2$ (1M) and $(NH_4)_2HPO_4$ (0.6M) solutions at pH 11 keeping with NH_4OH, followed by 24h maturation and 10h drying at 90ºC; (2) sintering at 1100ºC for 1h; and (3) grounding in agate planetary ball mill for 40 h. The defects were filled with composite paste containing nano-hydrohyapatite/3% solution of chitosan in citric acid, and electrospinning fibers of polylactic acid. After 84 days, histological and serum biochemical evaluation of the material showed that it is useful for repairing of critical calvarial defects. Acute and chronic inflammation or foreign body reaction was absented.

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P.S.E.3.

Biomimetic approach for preparation of calcium phosphate based cements

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Double-doped (with Mg^{2+} and Zn^{2+}) amorphous calcium phosphates (ACP) with molar ratios $(Ca^{2++}Mg^{2++}Zn^{2+})/P$ = 1.4 - 1.6, $Mg^{2+}/(Ca^{2++}Mg^{2++}Zn^{2+})$ = 0.8 - 0.14 and $Zn^{2+}/(Ca^{2++}Mg^{2++}\ Zn^{2+})$ = 0.017 – 0.029 were biomimetically (in the present of modified simulated body fluid and glycine) synthesized and used as a cement solid precursor. 18% solutions of three biocompatible carboxylic acids, namely citric acid, tartaric acid and lactic acid, were used as a liquid phase for the cements preparation. The effect of the acid used and of the solid to liquid ratio on the transformation of (Mg,Zn)-ACP to brushite phase and on forming characteristics, setting times, morphology and in vitro behavior of the obtained brushite cements were studied.

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P.S.E.4.

Corrosion behavior of nanotubular oxide layer formed on titanium and Ti–13Nb–13Zr alloy processed by high pressure torsion

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The good corrosion resistance is crucial for implant biomaterials application, because the metallic ion release from the implant to the surrounding tissue may give rise to biocompatibility problems. In order to optimize and enhance the implant material properties, the implant surfaces can be modified by different chemical surface treatments, including electrochemical anodic oxidation. In the present study nanotubular oxide layer on the surface of ultrafine-grained titanium (UFG cpTi), Ti-13Nb-13Zr (UFG TNZ) alloy and coarse-grained Ti-13Nb-13Zr (CG TNZ) alloy was formed using electrochemical anodization in 1M H_3PO_4 + 0.5 wt % NaF electrolyte, at room temperature during 60 minutes for UFG cpTi and 90 minutes for investigated alloys. The nanotubes morphology was studied using scanning electron microscopy (SEM). The SEM images showed that anodization of titanium and its alloy in a fluoride-containing electrolyte can lead to the formation of a highly regular self-organized nanotubular layer. Furthermore, nanotubes formed on UFG TNZ alloy were more uniformly arranged compared to nanotubes on CG TNZ alloy surface. The aim of this study was to determine the electrochemical behavior of titanium and its alloy after electrochemical anodization. Electrochemical measurements were performed in artificial saliva with a pH value of 5.5 at 37°C, in order to simulate the oral environment and examine the above-mentioned materials for dental application. The materials were analysed by electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization. All examined materials showed good corrosion resistance. The newly-formed inner barrier and outer porous surface layers were found to be highly resistant with capacitive behavior, but the materials with nanotubular oxide layer on their surface showed improved corrosion resistance.

P.S.E.5.

Effects of composition and method of preparation on biocompatible and biodegradable behavior of 3-D polymeric scaffolds based on gelatin/alginate/methacrylate

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Regenerative medicine focuses on repair/replacement of the damaged tissue or organ in our body. This is done by growing cells on scaffold materials which help in its attachment, migration and proliferation. Gelatin, a derivative of collagen, which is widely present in our body, is used as a component for promoting cell attachment, proliferation, and differentiation. Alginate, a naturally occurring polysaccharide contributes biocompatibility. Methacrylate based component improves strength and functional properties of scaffold. Biocompatible porous polymeric scaffolds provide a suitable environment for proliferation of cells in human body. In this research work, porous gelatin/alginate/methacrylate based scaffolds were prepared using porogen and freeze-gelation methods. Effects of parameters such as altering of composition and method of preparation on biocompatibility and biodegradation of scaffolds were investigated. The all synthesized scaffolds showed excellent biocompatible behavior evaluated by lactate dehydrogenase (LDH) activity. In vitro degradation study, performed during four months, indicates satisfactory degradation profile. It can conclude that obtained scaffolds possess versatile potentials in the field of biomedical engineering.

P.S.E.6.

Composite nanostructured HAp/YSZ dental inserts – processing, mechanical properties and application in dental restorations

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Bioceramic dental inserts reduce polymerization shrinkage and affect mechanical properties of the insert-containing dental restorations. The aim of this study was to investigate the sintering conditions of composite nano-powder based on hydroxyapatite (HAp) and yttrium-stabilized ZrO_2 (YSZ) in order to optimize microstructure, fracture toughness, hardness and shear bond strength (SBS) between processed composite inserts and restorative materials. Composite powder obtained by mixing 80 wt. % of stoichiometric HAp synthesized by modified precipitation method and 20 wt. % of YSZ synthesized by plasma method, after homogenization by ultrasound treatment were isostatically pressed into cylinder-shaped insert green bodies. After dilatometric analysis, HAp inserts were sintered in the temperature range of 1200°C-1325°C. Microstructural analysis of fractured surface showed the presence of two different fracture mechanisms due to YSZ addition, which affected fracture toughness and hardness increase. Sintering temperature and different application protocols significantly affected SBS between novel dentin substituents and commercial adhesive materials.

P.S.E.7.

Novel composite alginate hydrogels with activated charcoal as a carrier of therapeutically active substances

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In this work, we have produced novel composite alginate hydrogels containing activated charcoal (AC) particles that can carry one or more antimicrobial or therapeutically active substances and are released upon the contact with biological fluids over time. By varying concentrations of alginate (0.5 – 2 % w/w) and AC (1 – 20 % w/w) as well as gelation parameters (i.e. calcium and zinc cations, cation concentration and gelation time) the production method was optimized so that the obtained composite beads were releasing AC particles in the physiological saline solution over 5 days generally following the internal diffusion model. Furthermore, the composite beads with povidone iodine adsorbed onto AC have exhibited bactericidal effects against several bacterial strains. Thus the obtained composites are attractive for potential applications in wound treatments providing utilization of potent antiseptics such as iodine, without the concern that they will enter the body due to strong adsorption to AC.

P.S.E.8.

Towards a bio-nanoreactor by engineering inorganic nanoparticles with cancer cell membranes

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Biomimetic engineering has received an increasing interest to mimic biocompartmentalized enzyme regulatory mechanisms to design biomimetic nanomachineries with a potential in the range of biomedical applications. Therefore, mimicking the cellular biocompartment has triggered intensive research interest for creating new dynamic materials with tunable enzyme reactivity. Here, we aimed to develop a compartmentalized nanoreactor consisting of porous silicon nanoparticles entrapping horseradish peroxidase, and surface coated with a cancer cell membrane to demonstrate the design of biomimetic cellular nanoreactors and their impact on improving cellular functions for biomedical applications. The results suggest that the developed nanoreactors have high catalytic activity, cytocompatible, and readily integrated with cells. The intracellular activity of the nanoreactors showed significantly reduction of the intracellular ROS levels and supplemented the sub-cellular organelles' functions. Therefore, developed biomimetic nanoreactors can function as artificial organelles inside the cells to counteract the oxidative stress that is involved in an array of human diseases.

P.S.E.9.

Alumina based reinforcements for PMMA dental composite materials

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Poly(methyl metaacrilate) is one of widely used materials in dentistry and medicine mainly because of biocompatibility, inertness and possibility to be used in composite materials as a matrix. Fillers that are used in dentistry are mainly meant to improve the mechanical properties such as hardness, modulus of elasticity and stiffness as polymers sometimes don’t meet all the requirements.

Alumina is one of the fillers that exhibits important improvements in composite material. The chemical composition and crystal structure of the alumina can be modified trough additives and due to thermal treatment. There is also several routs to synthesize alumina based fillers and in this research the sol-gel based route starting from $Al_2Cl(OH)_5 \cdot 2,5H_2O$ as precursor was used. The chemical composition was modified by addition of Fe_2O_3. Three calcination temperatures 700° C, 800°C and 900°C were used in order to monitor the influence of this parameter to the composite properties.

The composites were made with the same amount of fillers and then the hardness of the obtained materials was measured. It was proved that the same concentration of the filler in the same matrix gave composites having important differences in mechanical properties. The hardness of the obtained composite having alumina fillers increased when fillers were treated at higher temperature. Also the modification of chemical composition of the filler using the Fe_2O_3 modifier gave even better improvement of the material harness.

P.S.E.10.

Comparative spectroscopic characterization of fullerene nanomaterials

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The higher fullerenes C76-D2 and C84-D2:22, as well as the basic fullerenes C60 and C70 were chromatographically isolated from carbon soot and the fullerol C60(OH)24 was synthesized, using new and advanced methods and processes. Their FT-IR(KBr) and electronic absorption spectra were recorded. All the observed infrared and UV/VIS bands are in excellent agreement with the theoretical calculations for these molecules. The molar absorptivity, as well as the integrated molar absorptivity of the absorption bands of the obtained fullerene nanomaterials was determined. These results are significant for their identification and quantitative determination either in natural resources or in artificially synthesized materials, electronic and optical devices, polymers, sensors, diagnostic and therapeutic agents, solar cells, nanophotonic lenses with optical absorption properties closer to human eye light sensitivity that can be used for early diagnosis of diabetes, in applied optical science, biomedical engineering and industry etc.

P.S.E.11.

3D finite elements modeling of the interfacial stresses bone/dental implant. Effects of the geometric parameters

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A successful osseointegration involves the simultaneous optimization of the primary stability of the implant and the minimization of interfacial stresses bone - implant. In this context, the modeling of these stresses has been given a great interest by researchers in last decades. The aim of this work is to study the effects of geometric parameters of a new model of titanium dental implant on the evolution of interfacial stresses bone /implant. For this, we have chosen a dental implant of the second premolar in the lower jaw, with different diameters, thread pitches and different thread forms. We have presented the profile of the interfacial stresses for each studied case, the results show a great similarity in the concerned areas, cortical bone, threaded region and cancellous bone, with the obtained results in the literature for other types of geometries.

Author Index

Peddis, Davide		66
Peeters, François M.		92
Penov-Gaši, Katarina M.		50
Peplińska, Barbara		47
Pérez-Murano, Francesc		56
Perić, Marko	markoperic1983@gmail.com	51, 81, 93, 94
Perović, Doug D.	doug.perovic@utoronto.ca	28
Pershin, Yuriy V.		46
Petriska, Martin		78
Petrović, Đorđe	djpetrovic@vin.bg.ac.rs	51, 81, 93, 94
Petrović, Tanja		69
Plyusnin, Pavel		44
Podchezertsev, Stanislav		65
Pokol, György		61
Poltarak, Anastasiia A.	poltarak.na@gmail.com	89
Poltarak, Pavel A.	poltarak_pa@mail.ru	89
Popa, Marcel I.		57
Popović, Zoran V.	popozor@ipb.ac.rs	40
Porfyrakis, Kyriakos		52
Postole, Georgeta		98
Predan, Felix		11
Prekajski Đorđević, Marija		45
Prespa, Edlira	prespaedlira@yahoo.com	43
Prlainović, Nevena		78
Rabadjieva, Diana		100
Rabasović, Maja S.		94
Radenović, Aleksandra	aleksandra.radenovic@epfl.ch	36
Radisavljević, Anđela		94
Radmilović, Velimir R.	vrradmilovic@lbl.gov,VRRadmilovic@tmf.bg.ac.rs	1, 53, 58, 95
Radmilović, Vuk V.	vukradmilovic@tmf.bg.ac.rs	53, 58, 95
Radojević, Vesna	vesnar@tmf.bg.ac.rs	85, 94, 106
Radović, Ljubica		69
Radović, Magdalena	magdalena.lazarevic@gmail.com	51, 81, 93, 94
Radović, Marko	marrad@biosense.rs	60
Rajh, Tijana	rajh@anl.gov	32
Rakić, Srđan		90
Rakić, Vesna	vesna.rakic@agrif.bg.ac.rs	98
Rakin, Marko P.		101
Rakonjac, Ivan		107
Raković, Dejan		84
Ramasse, Quentin M.	qmramasse@superstem.org	22

Zhu, Yimei	zhu@bnl.gov	38
Zlatanović, Miodrag	ezlatano@etf.rs	80
Zschech, Ehrenfried	ehrenfried.zschech@ikts.fraunhofer.de	23

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