NINETEENTH YOUNG RESEARCHERS' CONFERENCE MATERIALS SCIENCE AND ENGINEERING

December 1-3, 2021, Belgrade, Serbia

Program and the Book of Abstracts

Materials Research Society of Serbia &

Institute of Technical Sciences of SASA

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Aim of the Conference

Main aim of the conference is to enable young researchers (post-graduate, master or doctoral student, or a PhD holder younger than 35) working in the field of materials science and engineering, to meet their colleagues and exchange experiences about their research.

Topics

Biomaterials

Environmental science

Materials for high-technology applications Materials for new generation solar cells

Nanostructured materials

New synthesis and processing methods

Theoretical modelling of materials

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Results of the Conference

Beside printed «Program and the Book of Abstracts», which is disseminated to all conference participants, selected and awarded peer-reviewed papers will be published in journal "Tehnika – Novi Materijali". The best presented papers, suggested by Session Chairpersons and selected by Awards Committee, will be proclaimed at the Closing Ceremony. Part of the award is free-of-charge conference fee at YUCOMAT 2022.

Sponsors



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Programme Nineteenth Young Researchers Conference Materials Science and Engineering

Wednesday, December 1, 2021

09.00 – 10.15 1st Session – Biomaterials I Chairpersons: Prof. Dr. Bojana Obradović and Marija Kostić

$09.00-09.15\ Synthesis$ and characterization of the pH-sensitive saccharide-based polyurethane hydrogels

Marija Kostić

Faculty of Technology Novi Sad, University of Novi Sad, Novi Sad, Serbia

09.15 - 09.30 Antiradical activity of graphene quantum dots enriched albumin hydrogel: An EPR study

<u>Đura Nakarada</u>¹, Vladimir Trajković², Miloš Mojović¹

 $\overline{{}^{U}}$ University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia, 2 University of Belgrade, Faculty of Medicine, Belgrade, Serbia

09.30 – 09.45 Characterisctics of thin films of biological substances deposited on polyethylene terephthalate (PET) in terms of biomedical applications

K. Szafran¹, M. Jurak¹, R. Mroczka², A.E. Wiącek¹

¹Department of Interfacial Phenomena, Institute of Chemical Sciences, Faculty of Chemistry, Maria Curie-Skłodowska University, Lublin, POLAND, ²Laboratory of X-Ray Optics, Centre for Interdisciplinary Research, Faculty of Science and Health, The John Paul II Catholic University of Lublin, Poland

09.45-10.00 Additive-free resveratrol micro- and nanoparticles and assessment of their toxicity

Nina Tomić¹, Maja Kuzmanović¹, Dragana Mitić Ćulafić², Magdalena M. Stevanović¹

Institute of Technical Sciences of SASA, Knez Mihailova 35/IV 11000 Belgrade, Serbia,

Department of Microbiology, University of Belgrade - Faculty of Biology, Studentski trg 16, Belgrade, Serbia

10.00 - 10.15 The use of Langmuir's technique to assess the antibacterial properties of chemical substances

Agata Ładniak¹, Małgorzata Jurak¹, Marta Palusińska-Szysz², Klaudia Woźniak¹, Kacper Przykaza¹, Agnieszka Ewa Wiącek¹

¹Institute of Chemical Sciences, Department of Interfacial Phenomena, Faculty of Chemistry, Maria Curie-Skłodowska University, M.Curie-Skłodowska Sq. 3, 20-031 Lublin, Poland,

10.15 - 10.30 Break

10.30 – 12.00 2nd Session – Biomaterials II Chairpersons: Dr. Djordje Veljović and Ivana Banićević

10.30-10.45 Development of a physiologically relevant 3D in vitro model for osteosarcoma cell cultivation comprising alginate composite scaffolds and a perfusion bioreactor system

<u>Ivana Banićević</u>¹, Mia Radonjić¹, Marija Pavlović¹, Milena Milivojević², Milena Stevanović^{2,3,4}, Jasmina Stojkovska^{1,5}, Bojana Obradović¹

¹Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia, ²Institute of Molecular Genetics and Genetic Engineering, University of Belgrade, Belgrade, Serbia, ³Faculty of Biology, University of Belgrade, Belgrade, Serbia, ⁴Serbian Academy of Sciences and Arts, Belgrade, Serbia, ⁵Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia

10.45 – 11.00 Electrochemical composite bioceramic coatings based on hydroxyapatite, chitosan and polyvinyl alcohol loaded with gentamicin

Nevena Jaćimović¹, Marija Đošić², Ana Janković¹, Vesna Mišković – Stanković¹

Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, Belgrade, Serbia, ²Institute for Technology of Nuclear and Other Mineral Raw Materials, Bulevar Franš d'Eperea 86, Belgrade, Serbia

11.00 – 11.15 Optimization of Bioreactor Cultures of Glioblastoma Cells Immobilized in Alginate Microfibers

<u>Jelena Petrovic</u>^{1,2}, Mia Radonjic^{1,2}, Jasmina Stojkovska^{1,2}, Bojana Obradovic¹ *Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia,*²Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia

11.15-11.30 Laser induced periodic surface structures on Ti thin films by ultrafast laser irradiation

<u>Nevena Božinović</u>¹, Vladimir Rajić¹, Danilo Kisić¹, Dragana Tošić¹, Dubravka Milovanović², Suzana Petrović¹

¹Department of Atomic Physics, Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, P.O. Box 522, 11001 Belgrade, University of Belgrade, Serbia; ²University of Belgrade, Institute of General and Physical Chemistry, Studentski trg 12/V,11158 Belgrade, Serbia

²Institute of Biological Sciences, Department of Genetics and Microbiology, Faculty of Biology and Biotechnology, Maria Curie-Skłodowska University, Akademicka 19, 20-033 Lublin, Poland

11.30-11.45 Omitting mischmetal and zirconium as a next step in the development of biodegradable magnesium implants

Maria Zemkova¹, Peter Minarik¹, Eva Jablonska², Jozef Vesely¹, Jan Bohlen³, Robert Kral¹ Charles University, Ke Karlovu 5, 121 16 Prague, Czech Republic, ²University of Chemistry and Technology, Technicka 5, 166 28 Prague, Czech Republic, ³Helmholtz-Zentrum Geesthacht, Magnesium Innovation Center, Max-Planc-Straße 1, 215 02 Geesthacht, Germany

11.45 - 12.00 Photo-activation of a dental composite from within using optical fibers – a holographic study

<u>Evgenije Novta¹</u>, Tijana Lainović¹, Dušan Grujić², Svetlana Savić-Šević², Dejan Pantelić², Larisa Blažić^{1,3}

University of Novi Sad, Faculty of Medicine, School of Dental Medicine, Novi Sad, Serbia, University of Belgrade, Institute of Physics, Belgrade, Serbia, Dental Clinic of Vojvodina, Novi Sad, Serbia

12.00 - 12.15 Break

12.15 – 13.30 3rd Session – Biomaterials III

Chairpersons: Dr. Magdalena Stevanović and Tamara Matić

12.15 – 12.30 Electrophoretic deposition vs. dip-coating of the bioceramic layers on Ti6Al4V scaffolds

<u>Marija Milivojević</u>¹, Željko Radovanović¹, Suzana Dimitrijević², Miljana Popović², Rada Petrović², Đorđe Veljović², Đorđe Janaćković²

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

12.30 – 12.45 Dental inserts based on calcium hydroxyapatite: The influence of cation doping

<u>Tamara Matić</u>¹, Maja Ležaja Zebić², Vesna Miletić³, Rada Petrović⁴, Đorđe Janaćković⁴, Đorđe Veljović⁴

¹University of Belgrade, Innovation Center of the Faculty of Technology and Metallurgy, Belgrade, Serbia, ²University of Belgrade, School of Dental Medicine, Belgrade, Serbia, ³The University of Sydney, Faculty of Medicine and Health, Sydney Dental School, Surry Hills NSW, Australia, ⁴University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia

12.45 - 13.00 Synthesis and antimicrobial properties of ZnO deposited on hydroxyapatite

Marija Stevanović¹, Rada Petrović², Đorđe Veljović², Suzana Dimitrijević², Đorđe Janaćković²

 1 Inovacioni Centar Tehnološko-metalurškog fakulteta u Beogradu d.o.o, 2 Tehnološko-metalurški fakultet Univerzitet u Beogradu

$13.00-13.15\ Processing\ of\ gelatine\ coated\ composite\ scaffolds\ based\ on\ magnesium\ and\ strontium\ doped\ hydroxyapatite\ and\ yttria-stabilised\ zicronium\ oxide$

Aleksa Galić¹, Tamara Matić², Nataša Obradović², Đorđe Veljović¹

¹University of Belgrade, Faculty of Technology and Metallurgy, Department of Inorganic Chemical Technologies, Karnegijeva 4, 11000 Belgrade, Serbia, ²Innovation Center of Faculty of Technology and Metallurgy, Karnegijeva 4, 11000 Belgrade, Serbia

13.15 - 13.30 Dissolving and water absorption ability of spray-dried willow gentian extract

<u>Miloš Jovanović</u>¹, Nada Ćujić-Nikolić¹, Zorica Drinić¹, Teodora Janković¹, Smilja Marković², Katarina Šavikin¹

¹Institute for Medicinal Plants Research "Dr. Josif Pančić", Tadeuša Košćuška 1, 11000 Belgrade, ²Institute of Technical Sciences of SASA, Knez Mihailova 35/IV, 11000 Belgrade

13.30 - 14.45 Lunch break

14.45 – 16.15 4th Session – Environmental Materials I Chairpersons: Dr. Smilja Marković and Dr. Konrad Terpiłowski

14.45 – 15.00 Hydrophobization, a method of monument protection

Joanna Podkościelna, Konrad Terpiłowski

Department of Interfacial Phenomena, Institute of Chemical Sciences, Faculty of Chemistry, Maria Curie Skłodowska University Lublin, Poland

15.00-15.15 Optimization of biodiesel production from waste cooking oil using waste-based CaO/zeolite catalyst

Stefan Pavlović, Dalibor Marinković, Miroslav Stanković

University of Belgrade, Institute of Chemistry, Technology, and Metallurgy-National Institute of Republic of Serbia, Njegoševa 12, 11000 Belgrade

15.15 – 15.30 Experimental determination of thermodynamic propreties and modeling of new choline based ionic liquids

Ivona Đorđević, Nikola Grozdanić, Ivona Radović

University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11120 Belgrade, Serbia

$15.30-15.45 \ Xy lanase\ production\ from\ \textit{Penicillium\ chrysogenum\ } and\ its\ application\ in\ degradation\ of\ agricultural\ waste$

Olivera Vukoičić, Nataša Šekuljica, Zorica Knežević-Jugović

University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11120 Belgrade, Serbia

15.45 – 16.00 Carbon material derived from viscose as adsorbent for chlorpyrifos Vedran Milanković¹, Tamara Lazarević – Pašti²

¹University of Belgrade, Faculty of Physical Chemistry, Studentski Trg 12, 11000 Belgrade, Serbia, ²University of Belgrade, VINČA Institute of Nuclear Sciences - National Institute of the Republic of Serbia, Mike Petrovica Alasa 12-14, 11000 Belgrade, Serbia.

$16.00-16.15\ Application\ of\ DInSAR\ Technology\ for\ Monitoring\ the\ Subsidence\ Induced\ by\ Salt\ Mining\ in\ Tuzla,\ Bosnia\ and\ Herzegovina$

Bojana Grujić, Žarko Grujić

University of Banja Luka, Faculty of Architecture, Civil Engineering and Geodesy, Banja Luka/Department of Civil Engineering

16.15 - 16.30 Break

16.30 – 18.00 5th Session – Environmental Materials II Chairpersons: Dr. Ana Stanković and Michał Chodkowski

16.30 - 16.45 Effective sorption of toxic brilliant green using lignocellulosic waste biomasses and derived biochar samples

<u>Anja Antanasković</u>¹, Zorica Lopičić¹, Tatjana Šoštarić¹, Jelena Milojković¹, Vladimir Adamović¹, Kristina Vučković², Milan Milivojević²

¹Institute for Technology of Nuclear and Other Mineral Raw Materials, Belgrade, Serbia, ²Faculty of Technology and Metallurgy, University of Belgrade, Serbia

16.45-17.00 Synthesis of Samarium and Zirconium-doped TiO_2 nanofibers with improved photocatalytic activity

<u>Sanita Ahmetović</u>¹, Zorka Ž. Vasiljević¹, Nikola Cvjetićanin², Jelena Vujančević³, Nenad B. Tadić⁴, Vladimir B. Pavlović⁵, Maria Vesna Nikolić¹

¹University of Belgrade – Institute for Multidisciplinary Research, Belgrade, Serbia, ²University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia, ³ITS SASA, Belgrade, Serbia, ⁴University of Belgrade, Faculty of Agriculture, Belgrade, Serbia

17.00 - 17.15 Investigation of biological activity of freeze-dryed goat whey with the addition of dry spices

<u>Mihailo Mladenović</u>, Marija Milić, Suzana Dimitrijević-Branković University of Belgrade, Faculty of Technology and Metallurgy, Department of Biochemical Engineering and Biotechnology

17.15 – 17.30 Europium-doped manganese tungstate for dual electrocatalytic activity

Andrej Kukuruzar¹, Slađana Savić¹, Filip Vlahović², Dalibor Stanković^{1,3}

¹University of Belgrade, Faculty of Chemistry, Studentski trg 12-16, 11000, Beograd, Serbia, ²Innovation Center of the Faculty of Chemistry, University of Belgrade, Serbia, ³'VINČA' Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia

17.30 – 17.45 Thermally activated pyrophyllite as ceramic membrane

<u>Katarina Tošić</u>¹, Bojana Paskaš Mamula¹, Nikola Novaković¹, Mirjana Medić Ilić¹, Igor Milanović¹, Silvana Dimitrijević², Jasmina Grbović Novaković¹

Centre of Excellence for Hydrogen and Renewable Energy, Vinča Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, POB 522 Belgrade, Serbia, ²The Mining and Metallurgy Institute Bor, Zeleni bulevar 35, 19210 Bor, Serbia

17.45 - 18.00 Effects of sulphur hexafluoride cold plasma hydrophobization on the polyoxymethylene surface

Michał Chodkowski¹, Zoltan Károly², Szilvia Klébert², Konrad Terpiłowski¹

Department of Interfacial Phenomena, Institute of Chemical Sciences, Faculty of Chemistry, Maria Curie-Skłodowska University in Lublin (UMCS), pl. Marii Curie-Skłodowskiej 3, 20-031 Lublin, Poland, ²Institute of Materials and Environmental Chemistry, Research Centre for Natural Sciences, Magyar tudósok körútja 2, H-1117 Budapest, Hungary

Thursday, December 2, 2021

09.00 – 10.30 6th Session – Nanostructured Materials I Chairpersons: Dr. Sonia Jovanović and Dr. Ivana Dinić

09.00 – 09.15 Effect of processing parameters on NaGdYF₄:Yb,Er UCNPs structural, morphological and optical properties

Ivana Dinic¹, Marina Vukovic², Marko Nikolic³ and Lidija Mancic¹

Institute of Technical Sciences of SASA, Belgrade, Serbia, ² Innovative Centre, Faculty of Chemistry Belgrade, University of Belgrade, Serbia, ³Photonic Center, Institute of Physics Belgrade, University of Belgrade, Serbia

09.15 – 09.30 Electrochemical synthesis of silver nanoparticles in poly(vinyl alcohol)based hydrogels and evaluation of their sizes by comparing experimental and simulated UV-visible spectra

Marko Opsenica, Katarina Nešović, Vesna Mišković-Stanković University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, Belgrade, Serbia

09.30 – 09.45 Radiation-chemical synthesis of antibacterial Ag-poly(vinyl alcohol)/poly(N-vinyl-2-pyrrolidone) nanocomposite hydrogels

Nikolina Nikolić, Jelena Spasojević, Aleksandra Radosavljević, Zorica Kačarević-Popović Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia

09.45 – 10.00 Synthesis of nano-sized NiMn₂O₄ by glycine nitrate and electrospinning processes and its pseudocapacitive behavior

Milena Dojčinović¹, Zorka Ž. Vasiljević¹, Nenad Tadić², Jugoslav Krstić³, Smilja Marković⁴, Matiaž Spreitzer⁵, Janez Kovač⁵, Maria Vesna Nikolić¹

¹University of Belgrade – Institute for Multidisciplinary Research, Belgrade, Serbia, ²University of Belgrade, Faculty of Physics, Belgrade, Serbia, ³University of Belgrade, IChTM, Belgrade, Serbia, ⁴ITS of SASA, Belgrade, Serbia, ⁵Institute Jožef Štefan, Ljubljana, Slovenia

10.00 – 10.15 Characterization of a new Yb³⁺/Er³⁺ doped SrGd₂O₄ up-conversion nanomaterial obtained via glycine-assisted combustion synthesis

<u>Tijana Stamenković</u>¹, Nadežda Radmilović¹, Marija Prekajski-Đorđević², Ivana Dinić³, Lidija Mančić³, Vesna Lojpur¹

²Department of Materials, Vinča Institute of Nuclear Sciences, National Institute of the

¹Department of Atomic Physics, Vinča Institute of Nuclear Sciences, National Institute of the Republic of Serbia, P.O. Box 522, 11001 Belgrade, University of Belgrade, Serbia,

Republic of Serbia, P.O. Box 522, 11001 Belgrade, University of Belgrade, Serbia, ³Institute of Technical Science of SASA, Knez-Mihailova 35/4, Belgrade, Serbia

10.15-10.30 Improving the compatibility of zirconium oxide nanoparticles and styrene-free polyester resin by coupling with vinyl functionalized silane

Jelena D. Gržetić¹, Slavko Mijatov¹, Marica Bogosavljević¹, Tihomir Kovačević¹, Saša Brzić¹

Military Technical Institute, Ratka Resanovića 1, Belgrade, Serbia

10.30 - 10.45 Break

10.45 – 12.30 7th Session – Nanostructured Materials II Chairpersons: Dr. Suzana Filipović and Željko Mravik

10.45-11.00 Graphene quantum dots with amino groups as a potential photoluminescent probe for Fe(III) ions

Slađana Dorontić¹, Olivera Marković², Duška Kleut¹ and Svetlana Jovanović¹

Vinča"-Institute of Nuclear sciences - National Institute of the Republic of Serbia,
University of Belgrade P.O. Box 522, 11001 Belgrade, Serbia, ²University of BelgradeInstitute of Chemistry, Technology and Metallurgy, Department of Chemistry, Njegoševa 12,
11000 Belgrade, Republic of Serbia

11.00-11.15 Nanocomposite graphene oxide/silver nanowires: structural and morphological analysis

Aleksandra Mišović¹, Danica Bajuk Bogdanović², Milica Budimir¹ and Svetlana Jovanović¹ "Vinča" Institute of Nuclear Sciences - National Institute of the Republic of Serbia, University of Belgrade, 11000 Belgrade, Serbia, ²Faculty of Physical Chemistry, University of Belgrade, 11158 Belgrade, Serbia

11.15 – 11.30 Investigation of the interaction of graphene oxide and 12-tungstophosphoric acid in aqueous suspensions

Milica Pejčić¹, Željko Mravik¹, Danica Bajuk-Bogdanović², Snežana Uskoković-Marković³, Bojana Nedić Vasiljević², Sonja Jovanović¹, Zoran Jovanović¹

Laboratory of Physics, Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia, ²Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia, ³Faculty of Pharmacy, University of Belgrade, Belgrade, Belgrade, Belgrade, Serbia

11.30 – 11.45 Surface, structural and electric properties of ion beam irradiated graphene oxide papers

<u>Željko Mravik</u>¹, Marko Gloginjić¹, Danica Bajuk-Bogdanović², Maria Vesna Nikolić³, Andrzej Olejniczak^{4,5}, Nemanja Gavrilov², Zoran Jovanović¹

 1 Center of Excellence for Hydrogen and Renewable Energy (CONVINCE). Laboratory of Physics, Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia, ²Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia, ³Institute for Multidisciplinary Research, University of Belgrade, Serbia, ⁴Flerov Laboratory of Nuclear Reactions, Joint Institute for Nuclear Research, Dubna, Moscow region, Russia, ⁵Faculty of Chemistry, Nicolaus Copernicus University, Toruń, Poland

11.45 – 12.00 Hydrothermal synthesis and characterization of composite of graphene oxide and cobalt ferrite doped with zink and gallium

Marija Grujičić^{1,2}, Ivana Stojković Simatović¹, Danica Bajuk Bogdanović¹, Zoran Jovanović², Željko Mravik², Sonja Jovanović²

¹Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia, ²"VINČA" Institute of Nuclear Sciences – National Institute of the Republic of Serbia. University of Belgrade, Belgrade, Serbia

12.00 – 12.15 Hybrid functional porous polymers, based on phosphazene and cage-like siloxane building blocks

Mikhail Soldatov¹, Anna Chernysheva¹, Hongzhi Liu², Sergei Kostjuk³

¹D. Mendeleev University of Chemical Technology of Russia, Moscow, Russian Federation, ²Shandong University, Jinan, People Republic of China, ³Belarussian State University, Minsk, Republic of Belarus

12.15 – 12.30 Recent Progress of Carbon Dots in Nanomedicine and Photocatalysis Yigun Zhou and Roger M. Leblanc University of Miami, USA

12.30 – 13.45 Lunch break

13.45 – 15.00 8th Session – Theoretical Modeling of Materials I Chairpersons: Dr. Miloš Milović and Marko Jelić

13.45 – 14.00 Structural, spectroscopic and quantum-chemical investigation of testosterone propionate

Nikola Ristivojević, Dušan Dimić

University of Belgrade-Faculty of Physical Chemistry, Studentski trg 12-16, 11000 Belgrade, Serbia

14.00 – 14.15 Spectroscopic and theoretic analysis of hydrocortisone – forensic aspects Andjela Gavran, Dusan Dimic

University of Belgrade-Faculty of Physical Chemistry, Studentski trg 12-16, 11000 Belgrade, Serbia

14.15 – 14.30 The role of defects in graphene for removal of toxic compounds – Theoretical analysis

Marko Jelić^{1,2}, Aleksandar Jovanović¹, Igor Pašti¹

¹Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia, 2Laboratory of Physics, Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia

14.30 – 14.45 A DFT study of the influence of chemical environment and boron concentration in boron-doped graphene on its reactivity

Milica S. Ritopečki, Ana S. Dobrota

University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia

14.45-15.00 Significant modulation of charge-transfer states properties in the biological assembly of the $d(TG_4T)$ sequence in crystal form

Branislav Milovanović, Milena Petković, Mihajlo Etinski University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia

15.00 – 15.15 Break

15.15 – 16.45 9th Session – Theoretical Modeling of Materials II Chairpersons: Dr. Marko Opačić and Jovana Vlahović

15.15 - 15.30 Nitrogen-doped graphene nanoribbons: DFT prospects for Al-ion battery application

Jovana Vlahović^{1,2}, Ana S. Dobrota¹, Natalia V. Skorodumova^{3,4}, Igor A. Pašti^{1,3}

¹University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia, ²University of Belgrade, Vinča Institute of Nuclear Sciences, Laboratory of Physics, Belgrade, Serbia, ³KTH-Royal Institute of Technology, School of Industrial Engineering and Management, Department of Materials Science and Engineering, Brinellvägen 23, Stockholm, 100 44, Sweden, ⁴Uppsala University, Department of Physics and Astronomy, Box 516, 751 20 Uppsala, Sweden

15.30-15.45 The possibility of achieving bound states in complex periodic potential of the Kronig-Penney type

<u>Jovana Obradović</u>, Jelena Radovanović, Vitomir Milanović School of Electrical Engineering, University of Belgrade, Bulevar kralja Aleksandra 73, 11120 Belgrade, Serbia

$15.45-16.00\ Comparison\ of\ numerical\ methods\ for\ solving\ the\ effective\ mass\\ Schrödinger\ equation\ for\ multilayer\ heterostructure\ applications$

Novak Stanojević, Jelena Radovanović, Vitomir Milanović

School of Electrical Engineering, University of Belgrade, Bulevar kralja Aleksandra 73, 11120 Belgrade, Serbia

${\bf 16.00-16.15\ Construction\ of\ Symmetry-adapted\ k.p\ Hamiltonians\ for\ semiconductor\ nanostructures}$

Milan Jocić, Nenad Vukmirović

Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

16.15 – 16.30 Application of nanomaterials in mechanical engineering

Đorđe Jovanović¹, Mladen Krstić², Branislav Milenković³

¹Mathematical institute of SASA, Kneza Mihaila 36, 11000, Belgrade, Department of Computer Science, ²Faculty of Mechanical and Civil Engineering, Dositejeva 19, 36000, Kraljevo, Department of Mechanical Engineering, Faculty of Applied Science, Dušana Popovića 22a, 18000, Niš, Department of Mechanical Engineering

16.30 - 16.45 Numerical study of coupled heat and moisture transfer in a finite wall: effect of wall material on transfer properties

Zahreddine Hafsi

Laboratory of Applied Fluids Mechanics Process and Environment Engineering, National Engineering School of Sfax, University of Sfax, Sfax 3038, Tunisia

Friday, December 3, 2021

09.00 – 10.30 10th Session – Materials for High-technology Application I Chairpersons: Dr. Dragana Jugović and Dr. Milica Vasić

09.00-09.15 Simply prepared Mg-V-O as potential cathode material for rechargeable aqueous magnesium ion batteries

Milica M. Vasić¹, Miloš Milović², Danica Bajuk Bogdanović¹, Milica Vujković¹

¹University of Belgrade - Faculty of Physical Chemistry, Belgrade, Serbia, ²Institute of Technical Sciences of SASA, Belgrade, Serbia

09.15 – 09.30 Layered CaV₂O₆ as promising electrode material for multivalent storage Tamara Petrović¹, Miloš Milović², Danica Bajuk-Bogdanović¹, Milica Vujković¹ Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia, ²Institute of Technical Sciences of SASA, Belgrade, Serbia

09.30 - 09.45 Wearable Graphene Sensor for Pulse Measurement

<u>Teodora Vićentić</u>¹, Milena Rašljić Rafajilović¹, Bojana Koteska², Ana Madevska Bogdanova², Igor Pašti ³and Marko Spasenović¹

¹Center for Microelectronic Technologies, Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Serbia, ²Faculty of Computer Science and Engineering, "Ss. Cyril and Methodius" University of Skopje, North Macedonia, ³Faculty of Physical Chemistry, University of Belgrade, Serbia

09.45-10.00 Oxygen sensor based on mechanochemically treated metal oxide semiconducting TiO_2 - CeO_2 mixture

<u>Jelena N. Stevanović</u>¹, Srđan Petrović¹, Dana Vasiljević-Radović¹, Katarina Cvetanović¹, Nenad Tadić², Lazar Rakoćević³, Milija Sarajlić¹

¹Institute of Chemistry, Technology and Metallurgy, Njegoševa 12, University of Belgrade, Belgrade, ²Faculty of Physics, Cara Dušana 13, University of Belgrade, Belgrade, ³Vinča Institute of Nuclear Science, Mike Petrovića Street 12-14, University of Belgrade, Belgrade

10.00-10.15 Improving the electrocatalytic activity of nickel for HER in alkaline media by galvanic exchange with rhodium

<u>Lazar Bijelić</u>, Aleksandar Jovanović, Igor Pašti *University of Belgrade – Faculty of Physical Chemistry, Belgrade, Serbia*

10.15 – 10.30 Hydrogen evolution on graphene supported PtAu nanoparticles<u>Lazar Rakočević</u>¹, Ivana Stojković-Simatović², Aleksandar Maksić¹, Vladimir Rajić¹, Svetlana Štrbac³, Irina Srejić¹

¹INN Vinca, Laboratory of Atomic Physics, University of Belgrade, Serbia, Mike Alasa 12-14, 11001 Belgrade, Serbia, ²Faculty of Physical Chemistry, University of Belgrade, Serbia,

Studentski trg 12-16, 11158 Beograd, Serbia, ³Institute of Chemistry, Technology and Metallurgy, Department of Electrochemistry, University of Belgrade, Njegoševa 12, 11000 Belgrade, Serbia

10.30 – 10.45 Break

10.45 – 12.15 11th Session – Materials for High-technology Application II Chairpersons: Dr. Zoran Jovanović and Vladimir Terek

10.45 – 11.00 Electrochemical deposition for advanced engineering of novel electrocatalytic interfaces

Aleksandar Z. Jovanović¹, Sanjin J. Gutić², Lidija Rafailović³, Igor A. Pašti¹

¹University of Belgrade – Faculty of Physical Chemistry, Belgrade, Serbia, ²University of Sarajevo, Faculty of Science, Department of Chemistry, Sarajevo, Bosnia and Herzegovina, ³CEST, Centre of Electrochemical Surface Technology, Wr. Neustadt, Austria

11.00 – 11.15 Effect of different cobalt loadings on the electrochemical performance of aluminum pillared clay-supported cobalt towards glucose oxidation

<u>Biljana Milovanović</u>, Tihana Mudrinić, Sanja Marinović, Marija Ajduković, Aleksandra Milutinović-Nikolić, Predrag Banković

University of Belgrade - Institute of Chemistry, Technology and Metallurgy, National Institute of the Republic of Serbia, Department of Catalysis and Chemical Engineering, Njegoševa 12, Belgrade, Serbia

11.15-11.30 Synthesis and characterization of new dysprosium doped phosphate-tungsten bronze

<u>Tijana Maksimović</u>¹, Jelena Maksimović², Pavle Tančić³, Ljubinka Joksović¹, Maja Pagnacco⁴, Zoran Nedić²

¹Faculty of Science, Department of Chemistry, University of Kragujevac, Radoja Domanovića 12, 34000 Kragujevac, Serbia, ²Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12-16, 11001 Belgrade, Serbia, ³Geological Survey of Serbia, Rovinjska 12, 11000 Belgrade, Serbia, ⁴Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 12, 11000 Belgrade, Serbia

11.30 – 11.45 Novel PAN-based Air Filters for Potential Applications in Industrial Air Filtering and Facemask Production

<u>Mihailo Mirković</u>¹, Dušica Stojanović¹, Daniel Mijailović², Nemanja Barać², Đorđe Janaćković¹, Petar Uskoković¹

¹University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11120 Belgrade, Serbia, ²Innovation Center of Faculty of Technology and Metallurgy in Belgrade Ltd., Karnegijeva 4, 11120 Belgrade, Serbia

11.45 – 12.00 High temperature tribological testings of TiAlN coating

<u>Vladimir Terek</u>¹, Lazar Kovačević¹, Aleksandar Miletić², Branko Škorić^T, Aljaž Drnovšek³, Zoran Bobić¹, Pal Terek¹

¹University of Novi Sad, Faculty of Technical Sciences, Department of Production Engineering, Novi Sad, Serbia, ²Polytechnique Montreal, Department of Engineering Physics, Quebec, Canada, ³Jožef Stefan Institute, Department of Thin Films and Surfaces Ljubljana, Slovenia

12.00 - 12.15 Effects of corrosion on NiTi caused by fluoride and chloride media in non-accelerated corrosion tests

<u>Zoran Bobić</u>¹, Bojan Petrović², Sanja Kojić¹, Vladimir Terek¹, Lazar Kovačević¹, Goran Stojanović¹, Branko Škorić¹, Pal Terek¹

¹University of Novi Sad, Faculty of Technical Sciences, Department of production Engineering, Novi Sad, Serbia, ²University of Novi Sad, Faculty of Medicine, Novi Sad, Serbia

12.15 - 13.15 Lunch break

13.15 – 14.45 12th Session – Materials for High-technology Application III Chairpersons: Prof. Dr. Liiliana Damianović-Vasilić and S. Diurdiić Mijin

13.15 – 13.30 Raman Spectroscopy of Quasi-two-dimensional transition metal trihalides S. Djurdjić Mijin¹, AM Milinda Abeykoon², A. Solajić¹, A. Milosavljević¹, J. Pešić¹, M. Šćcepanović¹, Y. Liu³, A. Baum^{4,5}, C. Petrovic³, N. Lazarević₁, Z. V Popović^{1,6}

¹Center for Solid State Physics and New Materials, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia, ²National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, New York 11973, ³Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973-5000, United States, ⁴Walther Meissner Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany, ⁵Fakultat fur Physik E23, Technische Universit at Munchen, 85748 Garching, Germany, ⁶Serbian Academy of Sciences and Arts, Knez Mihailova 35, 11000 Belgrade, Serbia

13.30 – 13.45 Finishing of polyamide fabric with some boron compounds

Milena Nikodijević, Čedomir Dimić, Ivana Petrović, Dragan Đorđević Faculty of Technology, University of Niš

13.45 – 14.00 Zeolite-containing photocatalysts immobilized on aluminum support by plasma electrolytic oxidation

Kristina Mojsilović¹, Nikola Božović^{1,2}, Srna Stojanović³, Ljiljana Damjanović-Vasilić³, Maria Serdechnova⁴, Carsten Blawert⁴, Mikhail L. Zheludkevich^{4,5}, Stevan Stojadinović¹, Rastko Vasilić¹

¹Faculty of Physics, University Of Belgrade, Studentski trg 12-16, Belgrade 11000, Serbia, ²Directorate of Measures and Precious Metals, Mike Alasa 14, Belgrade 11000, Serbia, ³Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12-16, Belgrade 11000, Serbia, ⁴Institute of Surface Science, Hemholtz-Zentrum Hereon, Max-Plack-Straβe 1, Geesthacht 21502, Germany, ⁵Institute of Materials Science, Faculty of Engineering, Kiel University, Kaiserstraβe 2, Kiel 24143, Germany

14.00 – 14.15 Obtaining of healthcare textiles based on viscose fabric with improved sorption properties

Matea Korica¹, Zdenka Peršin², Lidija Fras-Zemljič², Mirjana Kostić³

¹Innovation Center of Faculty of Technology and Metallurgy, University of Belgrade, Serbia, ²Institute of Engineering Materials and Design, Faculty of Mechanical Engineering, University of Maribor, Slovenia, ³Faculty of Technology and Metallurgy, University of Belgrade, Serbia

14.15 – 14.30 Lattice dynamics and magnetism in Fe_{3-x}GeTe₂

Ana Milosavljević¹, Andrijana Šolajić¹, Sanja Đurđić Mijin¹, Jelena Pešić¹, Bojana Višić¹, Yu Liu², Cedomir Petrovic², Zoran V. Popović^{1,3}, Nenad Lazarević¹

¹Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia, ²Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York 11973-5000, USA, ³Serbian Academy of Sciences and Arts, Knez Mihailova 35, 11000 Belgrade, Serbia

14.30 – 14.45 Design of a pump for shipping crude oil from an oil terminal in Cameroon Lotin Thierry, Bella Marie

University of Douala, Faculty of sciences P.O. Box 245 Douala, Cameroon

14.45 – 15.00 Break

15.00 – 16.45 13th Session – New Synthesis and Processing Methods and Matherials for New Generation Solar Cells Chairpersons: Prof. Dr. Ivana Stojković Simatović and Jelena Mitrić

15.00-15.15 Application of supercritical carbon dioxide for making perovskite photodiode

Milica Stefanović¹, Rada Petrović², Ivana Lukić², Jelena Vujančević³, Đorđe Janaćković²

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

15.15 - 15.30 Optimisaton of materials for enhancement of efficiency of Dye Sensitized Solar Cells

<u>Evgenija Milinković¹</u>, Katarina Cvetanović¹, Dana Vasiljević-Radović¹ and Dragomir Stanisavljev²

¹Centre of Microelectronic Technologies, Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoseva 12, 11060 Belgrade, Serbia, ²Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12-16, 11060 Belgrade, Serbia

15.30 – 15.45 Investigation of photo(electro)catalytic efficiency of $BaTi_{1-x}Sn_x$, ZnO and $ZnO@BaTi_{1-x}Sn_x$ (x=0,0.05,0.10) powders

<u>Katarina Aleksić</u>¹, Ivan Supić², Ivana Štojković Simatović², Ana Stanković¹, Smilja Marković¹

¹Institute of Technical Sciences of SASA, Belgrade, Serbia, ²Faculty of Physical Chemistry, University of Belgrade, Serbia

15.45 – 16.00 Thin film nanocomposites based on polyaniline and silver nanowires for optoelectronic applications

Jovan Lukić, Vuk V. Radmilović

Faculty of Technology and Metallurgy, University of Belgrade, Serbia

16.00 – 16.15 Surface phonons in YVO₄:Eu³⁺ nanopowders

<u>J. Mitrić</u>¹, N. Paunović¹, M. Mitrić³, J. Ćirković², M. Gilić¹, M. Romčević¹ and N. Romčević¹

¹Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia, ²Institute for Multidisciplinary Research, University of Belgrade, Kneza Višeslava 1a, 11030 Belgrade, Serbia, ³Institute Vinča, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia

16.15 – 16.30 Hydrothermal synthesis of hydroxyapatite on calcium-enriched natural and synthetic zeolite as a carrier

<u>Katarina Sokić</u>¹, Đorđe Veljović¹, Jelena Dikić², Jovica Stojanović³, Danijela Smiljanić³, Sanja Jevtić¹

¹Faculty of Technology and Metallurgy, University of Belgrade, Serbia, ²Innovation centre of the Faculty of Technology and Metallurgy, University of Belgrade, Serbia, ³Institute for Technology of Nuclear and Other Mineral Raw Materials, University of Belgrade, Serbia

16.30 – **16.45** Synthesis of linear and star-shaped oligoimides by high-temperature catalytic polycondensation in a benzoic acid melt according to the Bn + AB scheme A.E. Soldatova¹, A.Ya. Tsegelskaya¹, I. G. Abramov², A. Kh. Shakhnes³, O.V. Serushkina³, A. Herberg⁴, A.A. Kuznetsov¹

¹Enikolopov Institute of Synthetic Polymeric Materials, Moscow, Russia, ²Yaroslavl State Technical University, Yaroslavl, Russia, ³Zelinsky Institute of Organic Chemistry, Moscow, Russia, ⁴Paderborn University, Paderborn, Germany

16.50 Closing Ceremony

8-3

The role of defects in graphene for removal of toxic compounds – Theoretical analysis

Marko Jelić^{1,2}, Aleksandar Jovanović¹, Igor Pašti¹

¹Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia,

²Laboratory of Physics, Vinča Institute of Nuclear Sciences – National Institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia

Understanding the adsorption of pesticides and toxic gases on graphene has high importance for their degradation and removal. In the present study, the adsorption of different models of organophosphate pesticides (OPH3, OPF3, SPH3 and SPF3) and inorganic molecules (H2O and NH3) on perfect and defected graphene was examined by using the DFT method. Inspected systems were pristine, single-vacancy (SV), Stone-Wales (SW) and epoxy graphene. Pristine graphene exhibits great adsorption affinity towards OPH3 molecule, while it shows insignificant adsorption towards other examined species. The introduction of defects influences the reactivity of these molecules on the graphene surface. Among them, SV graphene showed the highest adsorption affinity for H2O, NH3, OPH3 and OPF3, while SW graphene showed the most suitable adsorption properties towards SPH3 and SPF3 molecules. The interaction between molecules and graphene was mostly physisorption except in the case of epoxy graphene where degradation of organophosphates occurred (Figure 1). This study suggests that graphene can be potentially used to remove environmental pollutants and pesticides' chemical degradation, while the surface chemistry of graphene should be carefully tailored for this application.

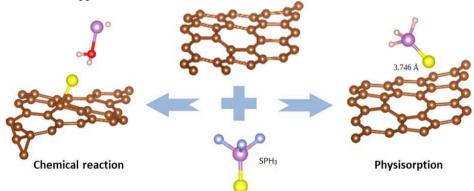


Figure 1. Schematic representation of the interaction between SPH3 molecule and the grapheme