

2nd International Meeting
on
MATERIALS SCIENCE FOR ENERGY RELATED APPLICATIONS
(Belgrade, September 29th-30th 2016)

Place: University of Belgrade, Faculty of Physical Chemistry, Studentski trg 12-16, Belgrade

Room: 368 (Amphitheatre)

P R O G R A M

DAY 1 – September 29th 2016

REGISTRATION and OPENING

8:00 to 9:00 Registration and posters mounting

9:00 to 9:10 **OPENING WORDS**

9:10 to 9:35 **PLENARY LECTURE** - Aleksandra Dapčević, LANTHANOIDE DOPED δ -Bi₂O₃ WITH ENHANCED CONDUCTIVITY

Session 1.1 – Solid electrolytes and oxide materials for energy related applications

9:40 to 9:55 V. Lutsyk, A. Zelenaya, M. Parfenova
 CRYSTALLIZATION PATHS IN CERAMIC SYSTEMS WITH THE MATERIALS FOR ENERGY APPLICATION

9:55 to 10:10 A.Radojković, M. Žunić, S.Savić, Z. Branković, G. Branković
 CHEMICAL STABILITY OF DOPED BaCe_{0.9}Y_{0.1}O_{3- δ} AS A PROTON CONDUCTING ELECTROLYTE FOR IT-SOFC

10:10 to 10:25 Olga Yu. Vekilova, Johan O. Nilsson, Johan Klarbring, Sergei I. Simak, Natalia V. Skorodumova
 IONIC CONDUCTIVITY IN DOPED CERIA FROM AB INITIO NON-EQUILIBRIUM MOLECULAR DYNAMICS COMBINED WITH A COLOR-DIFFUSION ALGORITHM

10:25 to 10:40 Johan O. Nilsson, Mikael Leetmaa, Olga Yu. Vekilova, Sergei I. Simak, and Natalia V. Skorodumova
 SIMULATION OF ION CONDUCTIVITY IN DOPED CERIA FROM FIRST PRINCIPLES

10:40 to 10:55 Sanja Pršić, Slavica M. Savić, Zorica Branković, Stanislav Vrtnik, Slavko Bernik and Goran Branković, THERMOELECTRIC PROPERTIES OF NaCo_{2-x}Cu_xO₄ (x = 0, 0.01, 0.03, 0.05) CERAMIC

Coffee break/Posters (10:55 to 11:25)

Session 1.2 – Heterogeneous catalysis and Photocatalysis

11:25 to 11:40 Ivana Lukić, Željka Kesić, Miodrag Zdujić, Dejan Skala
 SYNTHESIS OF METAL GLYCEROLATES AS CATALYSTS FOR BIODIESEL PRODUCTION

11:40 to 11:55 Jovana Ćirković, Danijela Luković Golić, Aleksandar Radojković, Aleksandra Dapčević, Zorica Branković, Goran Branković
 PHOTOCATALYTIC PROPERTIES OF BiFeO₃ PARTICLES SYNTHESIZED BY ULTRASOUND SOL-GEL ASSISTED ROUTE

11:55 to 12:10 T. D. Savić, M. I. Čomor, I. A. Janković, D. Ž. Veljković, S. D. Zarić
 SURFACE MODIFICATION OF ANATASE NANOPARTICLES MODIFIED WITH CATECHOLATE TYPE LIGANDS: EXPERIMENTAL AND DFT STUDY OF OPTICAL

	<i>PROPERTIES</i>
12:10 to 12:25	<u>Anton Kokalj</u> <i>A MODEL STUDY OF METHANE DEHYDROGENATION ON Rh@Cu(111)</i>
12:25 to 12:40	Vesna Đorđević, Jasmina Dostanić, Davor Lončarević, S. Phillip Ahrenkiel, Dušan N. Sredojević, Nenad Švrakić, <u>Jovan M. Nedeljković</u> <i>VISIBLE-LIGHT RESPONSIVE Al₂O₃ PARTICLES</i>
12:40 to 12:55	<u>Nikola Tasić</u> , Zorica Marinković Stanojević, Zorica Branković, Uroš Lačnjevac, Milan Žunić, Martina Gilić, Goran Branković <i>NANOSIZED ANATASE PARTICLES FOR APPLICATION IN DYE-SENSITIZED SOLAR CELLS (DSSCs)</i>
12:55 to 13:10	<u>Nikola Biliškov</u> , Danijela Vojta <i>IN-SITU TEMPERATURE DEPENDENT INFRARED SPECTROSCOPY OF AMMONIA BORANE DEHYDROGENATION</i>
Lunch/Posters (13:10 to 14:30) – (coffee will be served from 14:00 to 14:30)	
Session 1.3 – Surface processes	
14:30 to 14:45	<u>Aleksandar Z. Jovanović</u> <i>THEORETICAL ANALYSIS OF ADSORPTION PROPERTIES OF DOPED HEXAGONAL MgO NANOTUBES</i>
14:45 to 15:00	<u>Igor A. Pašti</u> , Natalia V. Skorodumova <i>CHANGING REACTIVITY OF SUPPORTED METAL ATOMS BY SUBSTRATE DOPING – THE CASE OF Pd AND Au ON DOPED MgO(001)</i>
15:00 to 15:15	<u>Katarina Batalović</u> , Igor Pašti, Jana Radaković, Carmen Rangel <i>MODIFYING THE SURFACE OF NITROGEN-DOPED TiO₂ PHOTOCATALYST WITH PALLADIUM AND PLATINUM</i>
15:15 to 15:30	<u>Aleksandra Marković</u> , Gunther Wittstock <i>SURFACE MODIFICATION BY SELF-ASSEMBLED MONOLAYERS OF FLUORESCENT DYES</i>
15:30 to 15:45	<u>M. Baljuzovic</u> , J. Girovsky, J. Nowakowski, Md. Ehesan Ali, H. R. Rossmann, T. Nijs, E. Aeby, S. Nowakowska, D. Siewert, G. Srivastava, C. Wäckerlin, J. Dreiser, S. Decurtins, Shi-Xia Liu, P. M. Oppeneer, T. A. Jung, N. Ballav <i>PHYSICS AND CHEMISTRY ON-SURFACES: INTERFACE MATERIALS CREATED VIA SURFACE ENGINEERING</i>
15:45 to 16:00	<u>Matic Poberžnik</u> , Anton Kokalj <i>ON THE ORIGIN OF SURPRISING ATTRACTIVE INTERACTIONS BETWEEN ELECTRONEGATIVE OXYGEN ADATOMS ON ALUMINUM SURFACES</i>
16:00 to 16:15	Johan O. Nilsson, Mikael Leetmaa, Baochang Wang, Pjotr Zguns, Anders Sandell, <u>Natalia V. Skorodumova</u> <i>KINETICS OF WATER ADSORPTION ON THE RUTILE TiO₂(110) SURFACE</i>
Coffee break (16:15 to 16:30)	
Session 1.4 – General session	
16:30 to 16:45	<u>Richard G. Compton</u> <i>NANO-IMPACTS: NEW INSIGHTS INTO NANOPARTICLES</i>
16:45 to 17:00	<u>V. Lutsyk</u> , V. Vorob'eva <i>4D PHASE DIAGRAMS FOR THE MOLTEN SALT REACTOR MATERIALS</i>
17:00 to 17:15	<u>Stanislav V. Sokolov</u> , Enno Kätelhön and Richard G. Compton <i>NEAR-WALL HINDERED DIFFUSION IN CONVECTIVE SYSTEMS: TRANSPORT LIMITATIONS IN COLLOIDAL AND NANOPARTICULATE SYSTEMS</i>

17:15 to 17:30	Seyed Ali Nabavi, Goran T. Vladislavljević, Vasilije Manović, <i>MANUFACTURING POLYMERIC CAPSULES FOR CO₂ CAPTURE USING MICROFLUIDIC EMULSIFICATION AND ON-THE-FLY PHOTOPOLYMERISATION</i>
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Social dinner (starts at 19:00)

DAY 2 – September 30th 2016

9:00 to 9:25	PLENARY LECTURE - Chris Batchelor-McAuley, <i>HYDROGEN OXIDATION: FROM THERMODYNAMICS TO THE REACTION KINETICS AT SINGLE NANOPARTICLES</i>
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Session 2.1 – Hydrogen storage, batteries and electrochemical capacitors

9:30 to 9:45	Anton Gradišek <i>BOROHYDRIDES AS HYDROGEN STORAGE MATERIALS: MOLECULAR DYNAMICS STUDIES</i>
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9:45 to 10:00	I. Milanovic, S. Milosevic, S. Kurko, M. Savic, R. Vujasin, A. Djukic, J. Grbovic Novakovic <i>INFLUENCE OF MILLING TIME ON HYDROGEN DESORPTION PROPERTIES OF LiAlH₄ – Fe₂O₃ COMPOSITE</i>
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10:00 to 10:15	Sandra Kurko, Radojka Vujasin, Bojana Paskaš Mamula, Jasmina Grbović Novaković and Nikola Novaković <i>DFT STUDY OF HYDROGEN DESORPTION PROPERTIES OF BORON DOPED MgH₂</i>
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10:15 to 10:30	Z. Jovanović, D. Bajuk-Bogdanović, M. Vujković, S. Jovanović, I. Holclajtner-Antunović <i>THE PHYSICO-CHEMICAL PROPERTIES OF GRAPHENE OXIDE – PHOSPHOTUNGSTIC ACID HYBRID CAPACITOR</i>
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10:30 to 10:45	Milica Vujković, Slavko Mentus <i>FARADAIC VERSUS PSEUDOCAPACITANCE MECHANISM OF CHARGE STORAGE IN NaFe_{0.95}V_{0.05}PO₄/C COMPOSITE</i>
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10:45 to 11:00	Sanja Milošević, Ivana Stojković Simatović, Sandra Kurko, Jasmina Grbović Novaković, Nikola Cvjetičanin <i>VO₂ POLYMORPH B AS A ELECTRODE MATERIAL IN ORGANIC AND AQUEOUS LI-ION BATTERIES</i>
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Coffee break/Posters (11:00 to 11:30)

Session 2.2 – Theory

11:30 to 11:45	Milijana Savić, Jana Radaković, Katarina Batalović <i>ELECTRONIC STRUCTURE INVESTIGATION OF AlH₃ POLYMORPHS</i>
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11:45 to 12:00	Sergei I. Simak <i>MATERIALS AT HIGH TEMPERATURES: A FIRST-PRINCIPLES THEORY</i>
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12:00 to 12:15	Jana Radaković, Katarina Batalović, Milijana Savić <i>THERMODYNAMICS AND FORMATION MECHANISM OF Gd_{0.5}M_{0.5}Cu₅ (M=Mg, Ca) ALLOY FROM FIRST PRINCIPLES</i>
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12:15 to 12:30	A. V. Ruban <i>STRUCTURAL AND ATOMIC CONFIGURATIONAL ASPECTS OF Cu₃Pt CATALYSTS</i>
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Lunch/Posters (12:30 to 14:00) (coffee will be served from 13:30 to 14:00)

Session 2.3 – Electrocatalysis

14:00 to 14:15	Milica Vasić, Maria Čebela, Radmila Hercigonja, Diogo M. F. Santos, Biljana Šljukić
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	<i>Pd-MODIFIED X ZEOLITE ELECTRODES FOR HYDROGEN EVOLUTION REACTION IN ALKALINE MEDIUM</i>
14:15 to 14:30	<u>Sanjin Gutić, Ana S. Dobrota, Igor A. Pašti</u> <i>SIMULTANEOUS ELECTROCHEMICAL REDUCTION OF GRAPHENE OXIDE AND DEPOSITION OF NICKEL: EFFECT OF REDUCTION TIME ON CATALYTIC PROPERTIES TOWARDS THE HYDROGEN EVOLUTION REACTION</i>
14:30 to 14:45	<u>Dragana D. Vasić Aničijević, Sladjana Lj. Maslovara, Vladimir M. Nikolić, Milica P. Marčeta Kaninski</u> <i>IMPROVED HER ACTIVITY OF Ni CATHODE ACTIVATED BY NiCoMo IONIC ACTIVATOR – A DFT ASPECT</i>
14:45 to 15:00	<u>Urša Petek, Francisco Ruiz-Zepeda, Martin Šala, Primož Jovanovič, Jonas Pampel, Tim Patrick Fellingner, Vid Simon Šelih, Marjan Bele, Miran Gaberšček</u> <i>THE ROLE OF METAL IMPURITIES IN THE ELECTROCATALYTIC PERFORMANCE OF NITROGEN-DOPED CARBON MATERIAL</i>
15:00 to 15:15	<u>Nikola Zdolšek, Aleksandra Dimitrijević, Tatjana Trtić-Petrović, Jugoslav Krstić, Danica Bajuk-Bogdanović, Biljana Šljukić</u> <i>FROM GREEN SOLVENT TO CARBON MATERIAL: APPLICATION OF IONIC LIQUID DERIVED CARBON FOR OXYGEN REDUCTION</i>
15:15 to 15:30	<u>Nemanja Gavrilov, Miloš Stevanović, Igor Pašti, Slavko Mentus</u> <i>INFLUENCE OF NON-AQUEOUS SOLVENTS ON ORR ELECTROCHEMISTRY</i>
15:30 to 15:45	<u>Viktor Čolić, Aliaksandr Bandarenka</u> <i>Pt-ALLOY ELECTROCATALYSTS FOR THE OXYGEN REDUCTION REACTION: FROM MODEL SURFACES TO NANOSTRUCTURED SYSTEMS</i>
Coffee break/Posters (15:45 to 16:15)	
Session 2.4 – Electrocatalyst stability/DURAPEM session	
16:15 to 16:30	<u>A. Pavlišič, P. Jovanovič, V. S. Šelih, M. Šala, M. Bele, G. Dražić, I. Arčon, S. Hočevar, A. Kokalj, N. Hodnik, M. Gaberšček</u> <i>HOW TO IMPROVE THE STABILITY OF PLATINUM-BASED ELECTROCATALYSTS?</i>
16:30 to 16:45	<u>Nejc Hodnik, Primož Jovanovič, Matija Gatalo, Francisco Ruiz-Zepeda, Marjan Bele, Miran Gaberšček</u> <i>ADVANCED CHARACTERIZATION ELECTROCHEMICAL METHODS FOR STUDYING NANOPARTICLE ELECTROCATALYSTS STABILITY</i>
16:45 to 17:00	<u>Primož Jovanovič, Andraž Pavlišič, Vid Simon Šelih, Martin Šala, Samo Hočevar, Marjan Bele, Francisco Ruiz-Zepeda, Goran Dražić, Nejc Hodnik, Miran Gaberšček</u> <i>ELECTROCATALYSTS STABILITY INVESTIGATION BY ELECTROCHEMICAL FLOW CELL ANALYTICS</i>
17:00 to 17:15	<u>Matija Gatalo, Primož Jovanovič, Jan-Philipp Grote, Francisco Ruiz-Zepeda, Nejc Hodnik, Goran Dražić, Marjan Bele, Karl J.J. Mayrhofer, Miran Gaberšček</u> <i>TUNING THE STABILITY OF PtCu₃/C ORR ELECTROCATALYST WITH GOLD DECORATION AND GOLD DOPING</i>
17:15 to 17:30	<u>Ana S. Dobrota, Igor A. Pašti</u> <i>FIRST PRINCIPLES INSIGHTS INTO GRAPHENE ELECTRONIC AND CHEMICAL PROPERTIES MODIFICATION BY SUBSTITUTIONAL DOPING</i>
17:30 to 17:45	<u>Ivan Stoševski, Jelena Krstić, Zorica Kačarević-Popović, Ščepan Miljanić</u> <i>INVESTIGATION OF THE RADIOLITICALLY SYNTHESIZED Ag/C CATALYST AS A POTENTIAL CATHODE MATERIAL OF AN ALKALINE FUEL CELL USING NEWLY DESIGNED GAS-FLOW HALF-CELL</i>
CLOSING WORDS and DISCUSSIONS 17:45-OPEN	