

3rd INTERNATIONAL MEETING
on
MATERIALS SCIENCE FOR ENERGY RELATED APPLICATIONS

(Belgrade, 25-26 September 2018)

University of Belgrade, Faculty of Physical Chemistry, Studentski trg 12-16, Belgrade, Room 368 (Amphitheatre)

ORAL PRESENTATIONS
PROGRAM

DAY 1 – September 25th 2018

REGISTRATION & OPENING	
08:00 – 09:00	<i>Registration / posters mounting / coffee</i>
09:00 – 09:10	OPENING WORDS
09:10 – 09:40	PLENARY LECTURE: V.R. Radmilović ATOMISTIC PHENOMENA IN FUNCTIONAL OXIDE NANOWIRES FOR ENERGY RELATED APPLICATION
Session 1.1 – SOLID ELECTROLYTES AND OXIDE MATERIALS (Chairperson: A. Dapčević)	
09:40 – 09:55	<u>V. Ribić</u> , A. Dapčević, N. Skorodumova, A. Rečnik, D. Luković Golić, G. Branković STRUCTURE CHARACTERIZATION OF Gd DOPED BiFeO ₃
09:55 – 10:10	<u>B. Vasić</u> , Z. Konstantinović, R. Gajić, A. Pomar MECHANICAL MODIFICATION OF LOCAL ELECTRICAL PROPERTIES OF METAL-OXIDE BASED IONIC CONDUCTORS AT NANOSCALE
10:10 – 10:25	<u>K. Batalović</u> , J. Radaković, N. Bundaleski, I. Pašti EXPERIMENTAL AND THEORETICAL INSIGHTS ON CHARGE TRANSFER AND CLUSTER FORMATION IN CO-DOPED N-TiO ₂
10:25 – 10:40	<u>A. Gradišek</u> NMR STUDIES OF MOLECULAR DYNAMICS IN CLOSO-BORANES
10:40 – 11:10	Coffee break / posters
Session 1.2 – MATERIALS FOR ELECTROCHEMICAL CAPACITORS (Chairperson: N. Gavrilov)	
11:10 – 11:25	<u>S. Breitenbach</u> , C. Unterweger, C. Fürst, A. Walter Hassel PREPARATION AND CHARACTERIZATION OF BIO-BASED ACTIVATED CARBON MATERIALS FOR USE AS SUPERCAPACITOR ELECTRODES
11:25 – 11:40	<u>P. Bober</u> , J. Pflieger, I.A. Pašti, N. Gavrilov, M. Trchová, J. Stejskal CARBONIZED CONDUCTING POLYANILINE/POLY(VINYL ALCOHOL) AEROGELS DERIVED FROM CRYOGELS FOR ELECTROCHEMICAL CAPACITORS
11:40 – 11:55	<u>S.J. Gutić</u> , S. Sopčić, I.A. Pašti THE NATURE OF REDUCED GRAPHENE OXIDE CAPACITANCE FROM SCAN RATE DEPENDENCES: ADVANTAGES AND ISSUES
11:55 – 12:10	<u>Ž. Mravik</u> , D. Bajuk-Bogdanović, M. Vujković, S. Marković, J. Kovač, S. Jovanović, I. Holclajtner-Antunović, Z. Jovanović SYNERGIC ACTIVITY OF GRAPHENE OXIDE AND 12-TUNGSTOPHOSPHORIC ACID IN THEIR NANOCOMPOSITE FOR SUPERCAPACITOR APPLICATIONS
12:10 – 12:25	<u>D. Karačić</u> , S. Korać, I.A. Pašti, D. Sačer, S.J. Gutić ALKALI METAL CATIONS IN ELECTROCHEMICAL REDUCTION OF GRAPHENE OXIDE: EFFECTS ON CAPACITIVE PERFORMANCE
12:25 – 12:40	<u>A. Rakić</u> , J. Milikić, J. Krstić, B. Šljukić, I. Pašti, G. Ćirić-Marjanović THE INFLUENCE OF HYDROLYZED COLLAGEN ON CAPACITANCE PROPERTIES OF CARBONIZED POLYANILINE
12:40 – 12:50	Short coffee break

Session 1.3 – SOLAR ENERGY MATERIALS (Chairperson: K. Batalović)	
12:50 – 13:05	<u>J. Pflieger</u> , D. Rais, P. Toman (<i>invited talk</i>) SINGLET FISSION IN ORGANIC MOLECULES FOR HARVESTING SHORT WAVELENGTH LIGHT IN PHOTOVOLTAICS
13:05 – 13:20	<u>J. Belić</u> and L. Visscher COMPUTATIONAL OPTIMIZATION OF DYE-SENSITIZED SOLAR CELLS
13:20 – 13:35	<u>J. Kuliček</u> , P. Gemeiner, M. Omastová, M. Mičušík POLYMER BASED NANOCOMPOSITES AS COUNTER ELECTRODES IN SOLAR CELLS APPLICATIONS
13:35 – 14:45	LUNCH (Coffee will be served 14:15 – 14:45)
14:45 – 15:15	PLENARY LECTURE: <u>C.G. Grangvist</u> IN HARMONY WITH THE ENVIRONMENT: NEW MATERIALS AND DEVICES FOR HARNESSING NATURE'S ENERGY FLOWS
Session 1.4 – ELECTROCATALYSIS (Chairperson: B. Šljukić Paunković)	
15:15 – 15:30	<u>K. Stojanovski</u> , P. Jovanović, L. Moriau, M. Bele, N. Hodnik, M. Gaberšček DOPING OF TiON _x WITH VARIOUS ELEMENTS AS POTENTIAL SUPPORT FOR Ir OXYGEN EVOLUTION REACTION ELECTROCATALYST IN ACIDIC MEDIA
15:30 – 15:45	<u>L. Moriau</u> , M. Bele, F. Ruiz Zepeda, M. Gatalo, U. Petek, A. Vižintin, M. Gaberšček, N. Hodnik GRAPHENE/TiON _x /PtCuIrR AS BIFUNCTIONAL CATALYST FOR OXYGEN REDUCTION AND OXYGEN EVOLUTION REACTIONS FOR THE REGENERATIVE PEM FUEL CELL
15:45 – 16:00	<u>M.M. Vasić</u> , J. Milikić, L. Amaral, N. Cvjetičanin, D. Jugović, R. Hercigonja, B. Šljukić NiA AND NiX ZEOLITES AS ELECTROCATALYSTS FOR WATER SPLITTING IN ALKALINE MEDIA
16:00 – 16:15	<u>M. Gatalo</u> , F. Ruiz-Zepeda, P. Jovanović, N. Hodnik, M. Bele, M. Gaberšček REPRODUCIBLE WATER BASED GRAM SCALE SYNTHESIS OF HIGHLY ACTIVE PtCu ₃ /C OXYGEN REDUCTION REACTION ELECTROCATALYST VIA GALVANIC DISPLACEMENT REACTION
16:15 – 16:30	<u>E. Coy</u> , L. Yate, D.P. Valencia, W. Aperador, K. Siuzdak, P. Torruella, S. Estrade, K. Załęski, I. Iatsunskyi, F. Peiro, X. Zhang, J. Tejada, Y. Li, R.F. Ziolo TAILORING NANOCOMPOSITE CARBIDE ELECTRODES FOR EFFICIENT HYDROGEN EVOLUTION REACTION
16:30 – 16:40	Short coffee break
16:40 – 16:55	<u>M. Prokop</u> , R. Kodým, T. Bystroň, M. Paidar, K. Bouzek KINETICS OF Pt DISSOLUTION AT CONDITIONS CORRESPONDING TO HIGH- TEMPERATURE PEM FUEL CELL OPERATION
16:55 – 17:10	<u>M. Bele</u> , N. Hodnik, M. Gatalo, P. Jovanović, G. Dražič, F. Ruiz-Zepeda, M. Gaberšček, S. Hočevar SYNTHESIS OF HIGH PERFORMANCE Pt-SKIN PtCu ₃ /C INTERMETALLIC SHELL PEM-FC ELECTROCATALYST
17:10 – 17:25	M. Šabanović, <u>D. Metarapi</u> , I.A. Pašti, S.J. Gutić ELECTROCATALYTIC BEHAVIOR OF PULSE-DEPOSITED NICKEL/REDUCED GRAPHENE OXIDE COMPOSITES
17:25 – 17:40	A.Z. Jovanović, I. Pašti, T. Trišović, <u>L.D. Rafailović</u> Pd SURFACE FUNCTIONALIZATION OF HIGH-SURFACE-AREA TRANSITION METAL ELECTROCATALYSTS FOR FUEL CELL APPLICATIONS
19:00	Social dinner

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ORAL PRESENTATIONS PROGRAM

DAY 2 – September 26th 2018

09:00 – 09:30	PLENARY LECTURE: <u>N. Lopez</u> CHALLENGES IN THE MODELING OF OXIDES WITH CATALYTIC PROPERTIES
Session 2.1 – THEORETICAL MODELLING (Chairperson: <i>I. Pašti</i>)	
09:30 – 09:45	<u>M. Rellán-Piñero</u> and N. López DYNAMIC BEHAVIOR OF ELECTRONIC CONFIGURATION ON REDUCED α -MoO ₃ (010): A DFT STUDY
09:45 – 10:00	<u>A.S. Dobrota</u> , I.A. Pašti, N.V. Skorodumova HOW DOES GRAPHENE REACT TO STRESS?
10:00 – 10:15	<u>A.Z. Jovanović</u> and I.A. Pašti FIRST PRINCIPLES INVESTIGATION OF THE CHEMICAL PROPERTIES OF SUBSTITUTIONALLY DOPED AND MONOVACANT GRAPHENE
10:15 – 10:30	<u>N.V. Skorodumova</u> , P. Zhgun, A.V. Ruban DOPANT AND VACANCY DISTRIBUTION IN Gd-DOPED CERIA AND ITS INFLUENCE ON THE OXIDE PROPERTIES
10:30 – 10:45	<u>S.I. Simak</u> LATTICE DYNAMICS AND SUPERIONIC TRANSITION IN CeO ₂ FROM FIRST PRINCIPLES
10:45 – 11:00	<u>O. Vekilova</u> and N.V. Skorodumova EFFECT OF TEMPERATURE ON THE ENERGY BARRIERS FOR OXYGEN VACANCY DIFFUSION IN DOPED CERIA
11:00 – 11:30	Coffee break / posters
Session 2.2 – HETEROGENEOUS CATALYSIS (Chairperson: <i>M. Milojević-Rakić</i>)	
11:30 – 11:45	<u>A. Kokalj</u> , J.J. Corral-Pérez, A. Bansode, C.S. Praveen, H. Reymond, A. Comas-Vives, J. VandeVondele, C. Copéret, P. Rudolf von Rohr, A. Urakawa UNIQUE REACTIVITY OF SILVER ON SILICA IN CO ₂ HYDROGENATION TO FORMATES AND SUBSEQUENT ESTERIFICATION WITH METHANOL TO METHYL FORMATE
11:45 – 12:00	<u>R. García-Muelas</u> , Q. Li, N. López HYDROGEN PRODUCTION FROM ALCOHOLS REFORMING ON NOBLE METALS: INSIGHTS FROM MICROKINETIC MODELING AND DENSITY FUNCTIONAL THEORY
12:00 – 12:15	<u>K. Karajović</u> , Q. Li, N. López ROLE OF ENSEMBLE CONTROL IN ALKYNE SEMI-HYDROGENATION ON Ni _x P _y CATALYSTS
12:15 – 12:30	<u>M. Baljozovic</u> , A. Mairena, M. Parchau, M. Kaweckı, L. Bernard, C. Wäckerlin, K.-H. Ernst UNRAVELLING THE ROLE OF TRANSIENTLY PRODUCED HYDROGEN IN ON-SURFACE CHEMISTRY
12:30 – 12:45	<u>E. Fako</u> , M. Ortuño, N. Lopez SINGLE ATOM CATALYSIS: THE MISSING LINK BETWEEN HOMOGENEOUS AND HETEROGENEOUS CATALYSIS
12:45 – 13:00	<u>V. Babačić</u> , Y. Wang, M. Lewandowski DETERMINING THE WORK FUNCTION OF ULTRATHIN FeO(111) FILMS ON Ag(111) – THE POTENTIAL OXIDATION CATALYSTS
13:00 – 14:30	LUNCH (Coffee will be served 14:00 – 14:30)

14:30 – 15:00	<i>PLENARY LECTURE: B. Johansson</i> THE PROCEDURE BEHIND THE NOBEL PRIZE IN PHYSICS
Session 2.3 – GENERAL SESSION (<i>Chairperson: S. Simak</i>)	
15:00 – 15:15	<u>N. Hodnik</u> and P. Stražar (<i>invited talk</i>) ENVIRONMENTALLY FRIENDLY RHODIUM DISSOLUTION PROCESS WITH OZONE, HYDROGEN AND CARBON MONOXIDE FOR RECYCLING PURPOSES
15:15 – 15:30	<u>J. Senčanski</u> , S. Blagojević, I. Stojković Simatović AN EXAMINATION OF METHODS USED IN RECYCLING CATHODE MATERIAL FROM SPENT Li-ION BATTERIES
15:30 – 15:45	<u>A. Marković</u> , L. Buschbeck, J. Christoffers, G. Wittstock FLUORESCENT DYES FOR ELECTROCHEMICAL SENSING – ELECTROCHEMICAL ACTIVATION OF SELF-ASSEMBLED MONOLAYERS
15:45 – 16:00	<u>B. Babić</u> , A. Kalijadis, M. Nikolić, M. Gilić, B. Jelenković, B. Jokić VISCOSE BASED SHINING CARBON DOTS
16:00 – 16:15	<u>D.M. Djokić</u> QUANTUM YIELD COMPUTATION IN POLYMER-WRAPPED CARBON NANOTUBES
16:15 – 16:25	Short coffee break
Session 2.4 – SURFACE PROCESSES AND CORROSION (<i>Chairperson: A. Kokalj</i>)	
16:25 – 16:40	<u>N. Godja</u> , A. Schindel, A. Laskos “SURFACE MODIFICATION TECHNOLOGIES“ USING PLASMA ELECTROLYTIC OXIDATION
16:40 – 16:55	<u>I.C. Vladu</u> , J. Wosik, A. Stankovic ELECTROSPUN NANOFIBERS AND THEIR POTENTIAL FOR ENERGY RELATED APPLICATIONS
16:55 – 17:10	<u>I. Traxler</u> , G. Schimo-Aichhorn, A. Muhr, G. Luckeneder, H. Duchaczek, K.-H. Stellnberger, J. Faderl, D. Rudomilova, T. Prosek, A.W. Hassel, S. Hild HYDROGEN DETECTION IN HIGH STRENGTH STEELS WITH ATOMIC FORCE MICROSCOPY
17:10 – 17:25	<u>P. Velicsanyi</u> , J. Schodl, G. Faflek, K.-H. Stellnberger, J. Hagler, W. Pernkopf, S. Piontek, P. Keil, R. Fluch CHARACTERISATION OF CORROSION MECHANISMS OF DIFFERENT SORTS OF STEEL AND DIFFERENT CORROSION PROTECTIVE ORGANIC COATINGS
17:25 – 17:40	<u>P. Jovanovič</u> , M. Bele, M. Šala, F. Ruiz-Zepeda, G. Dražić, N. Zabukovec Logar, N. Hodnik, M. Gaberšček CORROSION PROTECTION OF PLATINUM-BASED ELECTROCATALYST BY RUTHENIUM SURFACE DECORATION
17:40 – 17:55	<u>M. Poberžnik</u> and A. Kokalj LATERAL INTERACTIONS BETWEEN ELECTRONEGATIVE ADATOMS ON METALLIC SURFACES
17:55 – OPEN	<i>CLOSING WORDS and DISCUSSIONS</i>

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POSTER PRESENTATIONS PROGRAM

A.M. Juma and B.Ž. Todorović

FOURIER TRANSFORM INFRARED SPECTROSCOPY OF THE KEROGEN FROM ANTHRACITE AT VRŠKA ČUKA (SERBIA)

B. Simović, A. Dapčević, Ž. Radovanović, A. Golubović, A. Matković, G. Branković

COMPARATIVE STUDY OF Ag/ZnO NANOPOWDERS OBTAINED BY SOLVOTHERMAL AND PRECIPITATION METHODS

I. Šeděnková, M. Trchová, J. Dybal, J. Stejskal

ENHANCED THERMAL STABILITY OF POLYANILINE FILM WITH DIBUTYL PHOSPHITE

I.M. Minisy, N. Gavrilov, U. Acharya, C. Unterweger, J. Stejskal, P. Bober

CARBONIZED POLYPYRROLE NANOTUBES COVERED WITH GLOBULAR, NANOFIBRILAR OR NANOTUBULAR POLYPYRROLE

U. Acharya, P. Bober, J. Stejskal, J. Pflieger

POLYPYRROLE/MOLYBDENUM DISULPHIDE COMPOSITE AS PROMISING MATERIAL FOR ENERGY STORAGE

F. Piana, R. Jambor, T. Řičica, J.M. Macak, J. Pflieger

INKJET PRINTABLE NANOCOMPOSITE POLY(2-CYANOETHYL VINYL ETHER) / BARIUM TITANATE MATERIAL FOR ENERGY HARVESTING APPLICATIONS

F. Ruiz-Zepeda, L. Noč, G. Kapun, I. Jerman

ANALYTICAL (S)TEM INVESTIGATION OF BLACK PIGMENT COATING FOR APPLICATIONS IN CONCENTRATED SOLAR POWER

S. Aškračić, Z.D. Dohčević-Mitrović, V.D. Araújo, M. Radović, G.R. Costa, M.I.B. Bernardi, M.G. Nikolić

INFLUENCE OF Co DOPING ON OPTICAL AND PHOTOCATALYTIC PERFORMANCES OF SnO_{2-δ} NANOCRYSTALS

B. Stojadinović, M. Radović, N. Tadić, S. Stojadinović, I. Belča, Z. Dohčević-Mitrović

STABILITY OF F-CENTER DEFECTS DURING THE THERMAL TREATMENT OF NANOCRYSTALLINE CeO_{2-y}

N. Zdošek, J. Milikić, S. Mentus, M. Bendova, T. Trtić-Petrović, B. Šljukić

METAL CONTAINING IONIC LIQUID – NEW PRECURSOR FOR NICKEL/CARBON COMPOSITE CATALYST FOR BOROHYDRIDE OXIDATION AND OXYGEN REDUCTION REACTION

B.M. Kočmaruk and I.A. Pašti

ADSORPTION OF DIMETHYL SULFOXIDE AND ITS EFFECTS ON ELECTROCHEMICAL BEHAVIOR OF POTENTIODYNAMICALLY DEPOSITED POLYCRYSTALLINE PALLADIUM – EXPERIMENTAL AND THEORETICAL ANALYSIS

J.R. Vlahović

ADSORPTION OF MULTIVALENT METAL ATOMS ON FUNCTIONALIZED SURFACES OF GRAPHENE

K. Novčić and I.A. Pašti

INTERACTION OF Li_xO_y SPECIES WITH CARBON MATERIALS – ANALYSIS OF THE EFFECT OF SURFACE FUNCTIONALIZATION

A. Hrnjić, S. Marinković, I.A. Pašti, S.J. Gutić
PALLADIUM/REDUCED GRAPHENE OXIDE COMPOSITES AS ELECTROCATALYSTS IN ELECTROCHEMICAL WATER SPLITTING

S. Marinković, A. Hrnjić, I.A. Pašti, S.J. Gutić
ENHANCING PERFORMANCE OF rGO/Zn HYBRID ELECTROCHEMICAL CAPACITOR BY CONTROLLED-POTENTIAL REDUCTION OF GRAPHENE OXIDE

S.M. Brkovic, V.M. Nikolic, G.S. Tasic, D.L. Zugic, M.P. Marceta Kaninski
ELECTROCHEMICAL INVESTIGATION OF NON-STOICHIOMETRIC TUNGSTEN OXIDE SUPPORTED Pt AND Ru ELECTROCATALYSTS FOR CO TOLERANCE IN PEM FC

M. Šabanović, D. Metarapi, I.A. Pašti, S.J. Gutić
ELECTROCATALYTIC BEHAVIOR OF PULSE-DEPOSITED NICKEL/REDUCED GRAPHENE OXIDE COMPOSITES

W. Gouveia, S. Eugénio, B. Šljukić, U. Demirci, M.F. Montemor, D.M.F. Santos
COBALT-BASED FOAMS CATALYZED NaBH₄ HYDROLYSIS FOR H₂ ON-DEMAND DEVICES: IN-SITU REACTIVATION METHOD

A. Šaponjić, D. Žugić, Đ. Šaponjić, S. Brković, M. Pijović, V. Nikolić, M. Kokunešoski
CATALYSTS SUPPORT MATERIALS BASED ON Co/Mo BIMETALLIC CARBIDES

D. Mladenović, Ž. Mravik, Z. Jovanović, Š. Miljanić
TESTING OF GRAPHENE OXIDE ENRICHED WITH NAFION AS A MATERIAL FOR FUEL CELL MEMBRANES

N.P. Diklić and I.A. Pašti
LATTICE SURFACE STRAIN EFFECTS ON METAL ADSORPTION ON MgO(001)

A.S. Dobrota, I.A. Pašti, N.V. Skorodumova
OXYGEN REDUCTION ON GRAPHENE: A DFT VIEW ON THE ROLE OF NITROGEN FUNCTIONALITIES

I.A. Pašti, B. Johansson, N.V. Skorodumova
VACANCY FORMATION IN NICKEL OXIDE STUDIED BY DFT+U AND HYBRID CALCULATIONS

N. Gavrilov
PREPARATION OF SUPERCAPACITORS FROM ALGINATE FILMS FORMED DIRECTLY ON ELECTRODE SURFACE
