

# 1 s t W O R K S H O P

o n

## MATERIALS SCIENCE FOR ENERGY RELATED APPLICATIONS

(Belgrade, September 26<sup>th</sup>-27<sup>th</sup> 2014)

**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 26<sup>th</sup> 2014

##### REGISTRATION and OPENING

8:00 to 9:00 Registration and posters mounting

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

##### Session 1.1 – Methods (Chairperson: Natalia V. Skorodumova)

9:10 to 9:30 Olga Yu. Vekilova, Johan O. Nilsson, Olle Hellman, Sergei I. Simak and Natalia V. Skorodumova  
*AB INITIO NON-EQUILIBRIUM MOLECULAR DYNAMICS COMBINED WITH COLOR-DIFFUSION ALGORITHM: A THEORETICAL STUDY OF IONIC CONDUCTIVITY IN OXIDES*

9:30 to 9:50 Mikael Leetmaa  
*THE KINETIC MONTE-CARLO APPROACH TO STUDY SLOW DIFFUSION PROCESSES IN ENERGY RELATED MATERIALS USING KMCLib*

9:50 to 10:10 Petar Laušević, Vladimir Nikolić, Milica Marčeta Kaninski, Predrag Pejović  
*MODELING OF ELECTROCHEMICAL DOUBLE-LAYER CAPACITORS*

10:10 to 10:30 Biljana Babić, Branko Matović  
*NEW SYNTHETIC PROCEDURE FOR NANOMETRIC CARBIDES*

##### Coffee break/Posters (10:30 to 11:00)

##### Session 1.2 – Solid electrolytes and oxide materials for energy related applications (Chairperson: Dragana Jugović)

11:00 to 11:20 Anton Kokalj, Robert Dominko, Gregor Mali, Anton Meden, Miran Gaberšček, and Janez Jamnik  
*DESIGNING  $Li_2Mn_xFe_{1-x}SiO_4$  AS A POTENTIAL Li-BATTERY CATHODE MATERIAL*

11:20 to 11:40 Milica Vujković, Slavko Mentus  
*LITHIUM vs. SODIUM INTERCALATION MATERIALS IN AQUEOUS SOLUTIONS*

11:40 to 12:00 O. Hellman, N. V. Skorodumova and S. I. Simak  
*TUNING IONIC CONDUCTIVITY IN CERIA BY VOLUME OPTIMIZATION*

12:00 to 12:20 Johan O. Nilsson, Olga Yu. Vekilova, Olle Hellman, Sergei I. Simak, and Natalia V. Skorodumova  
*IONIC CONDUCTION IN GADOLINIUM-DOPED CERIA*

**Short coffee break (12:20 to 12:30)**

12:30 to 12:50 M. Prekajski, B. Matović, M. Stojmenović, G. Branković  
*SYNTHESIS AND CHARACTERIZATION OF  $Ce_{1-x}Bi_xO_{2-\delta}$  SOLID SOLUTION FOR SOLID OXIDE FUEL CELLS APPLICATION*

12:50 to 13:10 Yu.V. Pogorenko, R.M. Pshenychnyi, A.O. Omelchuk, V.I. Lutsyk  
*NOVEL FLUORINE-CONDUCTING SOLID ELECTROLYTES OF FLUORITE STRUCTURE IN THE  $KYF_4-PbF_2$  SYSTEM*

13:10 to 13:30 Natalia V. Skorodumova  
*FORMATION AND MOBILITY OF POLARONS IN OXIDES*

**Lunch/Posters (13:30 to 14:30)**

**Session 1.3 – Electrocatalysis (Chairperson: Igor Pašti)**

14:30 to 14:50 Debabrata Chanda, Jaromír Hnát, Martin Paidar, Karel Bouzek  
 *$NiFe_2O_4$  ELECTROCATALYST FOR THE HYDROGEN EVOLUTION IN ALKALINE WATER ELECTROLYSIS*

14:50 to 15:10 Dragana D. Vasić Aničijević, Vladimir M. Nikolić, Milica P. Marčeta-Kaninski and Igor A. Pašti  
*METAL OVERLAYER/TUNGSTEN CARBIDE HER ELECTROCATALYST: ELECTRONIC STRUCTURE AND THE SYNERGISM – A DFT APPROACH*

15:30 to 15:50 D.M.F. Santos, S. Eugénio, D.S.P. Cardoso, B. Šljukić, and M.F. Montemor  
*BOROHYDRIDE OXIDATION AT Ni-Cu NANOSTRUCTURED FOAMS*

15:50 to 16:10 Nemanja Gavrilov, Igor Pašti, Milan Momčilović, Marija Stojmenović, Biljana Babić, Slavko Mentus  
*EXPLORATION OF FACTORS GUIDING ORR ACTIVITY IN BORON DOPED ORDERED MESOPOROUS CARBONS*

**Short coffee break (16:10 to 16:20)**

16:20 to 16:40 Vladimir M. Nikolić, Ivana M. Perović, Danka D. Acimović, Biljana M. Babić, Igor A. Pašti, Milica P. Marčeta Kaninski  
*ON THE WAY OF IMPROVING CO TOLERANCE OF ANODE CATALYST IN PEM FUEL CELL*

16:40 to 17:00 Zdenka Stancic  
*SYNTHESIS OF Pd-Ni/C ELECTROCATALYST AND ITS ELECTROCATALYTIC ACTIVITY FOR ALCOHOLS OXIDATION IN ALKALINE MEDIA*

17:00 to 17:20 Petar Laušević, Vladimir Nikolić, Đorđe Šaponjić, Milica Marceta Kaninski  
*A LIFE TIME MODEL FOR PEM FUEL CELLS BASED ON VOLTAGE DEGRADATION*

**Dinner (starts at 19:00, Restaurant “Mali Vrabac”, Skadarlija)**

## DAY 2 – September 27<sup>th</sup> 2014

### Session 2.1 – Heterogeneous catalysis and Photocatalysis (Chairperson: Ljiljana Damjanović)

9:00 to 9:20	<u>I. Pašti</u> , L. P. Granda Marulanda, N. V. Skorodumova <i>SYSTEMATIC DFT STUDY OF BIMETALLIC DIMERS SUPPORTED BY MgO(001)</i>
9:20 to 9:40	<u>P. A. Žguncs</u> , I. Pašti, M. Wessel, N. V. Skorodumova <i>ADATOM CHARGING ON METAL SUPPORTED THIN FILMS: MECHANISM AND PERSPECTIVES FOR CATALYSIS</i>
9:40 to 10:00	<u>Ž. Kesić</u> , I. Lukić, <u>M. Zdujić</u> , Lj. Mojović, D. Skala <i>SYNTHESIS AND TESTING OF HETEROGENEOUS CATALYSTS FOR BIODIESEL</i>
10:00 to 10:20	Mina Medić, Aleksandra Zarubica, Scott P. Ahrenkiel, Vesna Lojpur, Ivana Vukoje, Miroslav D. Dramićanin, <u>Jovan M. Nedeljković</u> <i>PHOTOCATALYTIC PERFORMANCE OF Mg<sub>2</sub>TiO<sub>4</sub> NANOPOWDER</i>

### Coffee break/Posters (10:20 to 10:50)

### Session 2.2 – Hydrogen storage (Chairperson: Slavko Mentus)

10:50 to 11:10	<u>I. Milanović</u> , R. Vujasin, Lj. Matović, A. Đukić, B. Paskaš Mamula, J. Grbović Novaković and N. Novaković <i>HYDROGEN STORAGE PROPERTIES OF MgH<sub>2</sub> BASED HYDRIDES DOPED WITH SiC, TiB<sub>2</sub> AND LiAlH<sub>4</sub></i>
11:10 to 11:30	<u>S. Kurko</u> , R. Vujasin, Lj. Matović, A. Đukić, B. Paskaš Mamula, J. Grbović Novaković and N. Novaković <i>EFFECT OF VACANCIES ON HYDROGEN DESORPTION PROPERTIES OF MgH<sub>2</sub></i>
11:30 to 11:50	<u>S. Milošević</u> , R. Vujasin, S. Kumrić, Lj. Matović, Ž. Rašković-Lovre, L. Pasquini, J. Grbović Novaković <i>ENHANCED HYDROGEN SORPTION PROPERTIES OF MgH<sub>2</sub> CATALISED WITH VO<sub>2</sub>(B)</i>
11:50 to 12:10	<u>R. Vujasin</u> , B. Paskaš Mamula, I. Milanović, J. Grbović Novaković, N. Novaković <i>HYDROGEN DIFFUSION IN SURFACE AREA OF TiO<sub>2</sub></i>

### Short coffee break (12:10 to 12:20)

12:20 to 12:40	<u>D. Conić</u> , K. Batalović <i>KINETICS OF HYDROGEN ABSORPTION BY Zr-BASED ALLOYS BASED ON CHOU MODEL</i>
12:40 to 13:00	<u>Katarina Batalović</u> , Jana Radaković, Vasil Koteski <i>THERMODYNAMICS AND ELECTRONIC STRUCTURE OF HYDROGEN STORAGE MATERIALS – INSIGHT FROM DFT</i>
13:00 to 13:20	<u>Jana Radaković</u> , Katarina Batalović, and Jelena Belošević-Čavor <i>ELECTRONIC STRUCTURE AND STABILITY OF INTERSTITIAL MONOHYDRIDES</i>

### Closing words (13:20 to 13:30)

### Lunch/Posters (13:30 to 14:30)