















8 TINTERNATIONAL WORKSHOP OF MATERIALS PHYSICS

Magurele, Romania

National Institute of Materials Physics



Advanced Materials and Methods for Heterogeneous Catalysis

PROGRAM

Wednesday 17th of May 2023

| vvednes | wednesday, 17" of May 2023 | | |
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| 08:15 | Registration – Otetelesanu Mansion | | |
| 08:45 | Official opening – Mihaela Florea; Lucian Pintilie | | |
| Session | Session 1: Chairman – Mihaela Florea | | |
| 09:00 | Javier Garcia Martinez University of Alicante, Alicante, Spain Materials at order-discorder boundary: defect engineering for superior catalytic performance | | |
| 09:35 | Bao-Lian Su University of Namur, Namur, Belgium Natural laws for design of high performance hiererachically porous nanomaterials for energy storage and conversion | | |
| 10:10 | Radu Crăciun BASF Corp., New Jersey, USA Novelty and challenges in industrial catalysis | | |
| 10:45 | Coffee Break | | |
| 11.15 | Andrew Rappe University of Pennsylvania, Philadelphia, PA, USA New first-principles methods and insights into surface catalysis: reconstructions, pathways, and mechanochemistry | | |
| 11:50 | Leonarda Liotta Institute for the Study of Nanostructured Materials, Palermo, Italy Design of Ni based catalysts with tailored properties: investigation of the CO2 reforming of CH4 | | |
| 12:25 | Carmen Ciotonea Université du Littoral Côte d'Opale, Dunkerque, France Playing on the activity and selectivity of supported transition metal catalysts through metal dispersion: example in energy-related reactions | | |
| 13:00 | Lunch | | |

| Session | Session 2: Chairman – Florentina Neaţu | | |
|---------|--------------------------------------------------------------------------|--|--|
| | Michel Barsoum | | |
| 14:00 | Drexel University, Philadelphia, PA, USA | | |
| | Hydroxide derived nanomaterials and their properties | | |
| | Marius Andruh | | |
| 14:35 | Institute of Organic and Supramolecular Chemistry of the Romanian | | |
| 11.00 | Academy, Bucharest, Romania | | |
| | Metal-radical complexes in molecular magnetism | | |
| | Hui Luo | | |
| 15:10 | University of Surrey, Guildford, Surrey, UK | | |
| 10110 | Waste valorization with electrochemistry and mechanochemistry: towards | | |
| | sustainable Co-production of Hydrogen and value-added chemicals | | |
| | Aurelia Vișa | | |
| 15:45 | "Coriolan Dragulescu" Institute of Chemistry, Timisoara, Romania | | |
| | Metal(II) coordination polymers based on bisphosphonates or mixed | | |
| | imidazole ligands and bisphosphonates: green syntheses and applications | | |
| 16:05 | Coffee Break | | |
| | Alina Tomoiaga | | |
| 16:35 | European Innovation Council, Brussel, Belgium | | |
| 10.00 | The European Innovation Council: Funding opportunities for innovators to | | |
| | pursue their dreams | | |
| | Trends and new equipment | | |
| | Liana Socaciu-Siebert | | |
| 17:10 | SPECS Surface Nano Analysis GmbH, Berlin, Germany | | |
| 17:10 | NAP-XPS Instrumentation and Applications Ahmed DHIFAOUI | | |
| | JEOL (Europe) SAS France | | |
| | The new generation of JEOL NMR: ECZ Luminous Series | | |
| | | | |
| 18:00 | Posters Session | | |
| 20:00 | Dinner | | |

Thursday, 18th of May 2023

| ession 3: (| Chairman – Cristian M. Teodorescu |
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| | Paolo Fornasiero |
| 09:00 | University of Trieste, Trieste, Italy |
| | The metal/non-metal trajectory in sustainable chemistry |
| | Jeroen van Bokhoven |
| 09:35 | ETH Zürich and Paul Scherrer Institute, Zürich, Switzerland |
| | About the complexity of characterizing heterogeneous catalysts |
| 10:10 | Eric Altman Yale University, New Haven, Connecticut, USA |
| 10.10 | Non-contact atomic force microscopy as a tool for catalysis research |
| 10:45 | Coffee Break |
| 10.45 | |
| | Luca Artiglia Paul Schorrer Institute Villigen, Switzerland |
| 11.15 | Paul Scherrer Institute, Villigen, Switzerland In situ photoelectron spectroscopy studies of the structure-activity |
| | relationship |
| | Ruxandra Costescu |
| 44.50 | National Institute of Materials Physics, Magurele, Romania |
| 11:50 | Surface reactions and intercalation of carbon monoxide between |
| | graphene and Pt(001) |
| | Claudiu Colbea |
| 12:10 | ETH Zürich, Zürich, Switzerland |
| 12.10 | Surface chemistry by operando SEM and XPS |
| 12:30 | Lunch |
| ession 4: | Chairman – Ionuţ Enculescu |
| | Andras Tompos |
| 13:30 | Institute of Materials and Environmental Chemistry, Budapest, Hunga |
| 13.30 | Materials science in the development proton exchange membrane fu |
| | cell components: recent trends and new results |
| | Antonio Chaparro |
| 14:05 | CIEMAT, Department of Energy, Madrid, Spain |
| | Optimization of transport in gas-diffusion electrodes for proton- |
| | exchange membrane fuel cells |
| 14.40 | Dario Dekel |
| 14:40 | Technion – Israel Institute of Technology, Haifa, Israel |
| | Stability challenges of anion-exchange membranes Nicoleta Cioatera |
| 15:15 | University of Craiova, Craiova, Romania |
| | Electrocatalysts for a sustainable future |
| 10.10 | Libertocatary sto for a sustainable fatare |
| 10.10 | Ariana Serban |
| | Ariana Şerban École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland |
| 15:35 | École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland |
| | École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland |
| | École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland Enhancing water electrolysis efficiency through synergetic function o |

Friday, 19th of May 2023

Session 5: Chairman – Ştefan Neaţu

| Session 5: (| Session 5: Chairman – Ștefan Neațu | | |
|--------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--|--|
| 09:00 | Gregory Rohrer Carnegie Mellon University, Pittsburg, PA, US The influence of molten salts on SrTiO ₃ photocatalyst surfaces: surface restructuring and ion exchange | | |
| 09:35 | Gabriela Cârjă Technical University Gheorghe Asachi of Iasi, Iasi, Romania Engineering heterostructures of Zn-Based layered double hydroxides and gold nanoparticles for plasmon enhanced catalysis | | |
| 10:10 | Maria Miheţ National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania Ni-based catalysts with controlled porosity for gas phase CO ₂ conversion | | |
| 10:45 | Coffee Break | | |
| 11.15 | Cezar Comănescu National Institute of Materials Physics, Magurele, Romania Development of novel catalysts for enhanced hydrogen storage properties of complex hydrides | | |
| 11:35 | Crina Socaci National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania TiO ₂ /graphene-based nanomaterials to address the emerging contaminants pollution | | |
| 11:55 | Ştefan NăstaseKing Abdullah University of Science and Technology, Saudi ArabiaComputational study analyzing the effect of acid site proximity on themethanol to hydrocarbons process | | |
| 12:15 | Anca Păun University of Bucharest, Bucharest, Romania Thioorganic azoles in transition metal catalysed alkynylation reactions | | |
| 12:35 | Florentina Neaţu National Institute of Materials Physics, Magurele, Romania Modified 2D materials for plastic (PET) waste management | | |
| 12:55 | Concluding Remarks – Mihaela Florea; Ionuţ Enculescu | | |
| 13:05 | Lunch and departure | | |

Poster presentations

| P1 | Selective oxidation of p-cymene using MAX phase catalysts Iuliana M. Chirică, Mihaela M. Trandafir, Florentina Neaţu, Ştefan Neaţu, Michel W. Barsoum, Mihaela Florea |
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| P2 | Synthesis of N-acylhydrazone-based arylazopyrazoles and evaluation as multistate photoswitches George Costache, Bogdan C. Enache, Anamaria Hanganu, Codruţa Popescu, Anca Păun, Mihaela Matache |
| P3 | Novel perspectives of azo photoswitches: synthesis of oxa / thiadiazole decorated compounds and evaluation as switches Adela F. Dobre, Nicoleta Sandu, Anamaria Hanganu, Ioana Nicolau, Codruţa C. Popescu, Anca Păun, Augustin M. Mădălan, Mihaela Matache |
| P4 | Optimizing MXene-MoS ₂ semiconductor photocatalyst for water splitting Alexandra C. Iacoban, Mahesh M. Nair, Florentina Neaţu, Mihaela Florea, Ştefan Neaţu |
| P5 | Heterogeneous catalyst based on vinyl phosphonate in sustainable syntheses Bianca Maranescu, Aurelia Vișa |
| Р6 | NMR spectroscopy - a useful tool for monitoring formation of benfotiamine from thiamine Daniel P. Funeriu, Mihaela Matache, Maximov V. Maxim, Maximov Oana Cristina, Anamaria Hanganu, Codruţa Popescu, Nicoleta Sandu, Adela Dobre, Mihaela Florea |
| P7 | Slot-die coated perovskite solar cells: Effects of annealing temperature on performance of perovskite MAPbl _{2.6} Cl _{0.4} solar cells Anca G. Mirea, F. Neaţu, A. G. Tomulescu, L. Bălescu, M. Botea, M. Florea, I. Pintilie |
| Р8 | Synthesis of metal-based catalyst for the selective reduction of cinnamaldehyde Anca Gabriela Mirea, Maria-Iuliana Chirică, Ștefan Neaţu, Florentina Neaţu, Mihaela Florea, Mihaela-Mirela Trandafir |
| P9 | Surfactant assisted method for iron doped cobalt oxides preparation and their behavior in the oxidative transformation of malic acid Gheorghiţa Mitran, Mihaela Florea, Ştefan Neaţu, Florentina Neaţu |
| P10 | Influence of <i>i</i> -MXenes on the photocatalytic H ₂ evolution performance of TiO ₂ Mahesh M. Nair, Alexandra C. Iacoban, Florentina Neaţu, Mihaela Florea, Ștefan Neaţu |
| P11 | Polyurea coatings for military textiles Oana Hoza, Raluca Ginghină, Ciprian Său, Adriana Bratu, Gabriela Toader, Aurel Diacon, Iulian Vasile Antoniac, Nicoleta Petrea |
| P12 | Synthesis of novel benzimidazole-2-ones mediated by hypervalent iodine agent Maria Popescu, Anamaria Hanganu, Anca Păun, Ioana Nicolau, Mihaela Matache, Codruța Popescu |
| P13 | Synthesis of novel tricarboxylic units for hybrid organic-inorganic materials Nicoleta Sandu, Anca G. Mirea, Anamaria Hanganu, Mihaela Florea, Ioana Nicolau, Anca Păun, Codruța C. Popescu, Mihaela Matache |
| P14 | The effect of Ni deposition methods on SnO ₂ on the bioethanol electrooxidation performance Izabella Dascălu, Tanta Spătaru, Daniela C. Culita, Ștefan Neaţu, Florentina Neaţu, Mihaela Florea, Nicoleta Petrea, Vasile Somoghi, Simona Somăcescu |
| P15 | Oxide electrocatalysts based on non noble metals used as anodes for pemfcs working with bioethanol Mihaela Florea, Florentina Neaţu, Stefan Neaţu, Simona Somăcescu, Nicoleta Petrea, Doru-Gabriel Iosub, Vasile Somoghi |