BOOK OF ABSTRACTS



The 4th International Conference on Nanomaterials: Fundamentals and Applications

November 10-11, 2020 Online conference

Organized by:

Department of Physical Chemistry Faculty of Natural Science Pavol Jozef Šafárik University in Košice & Slovak Chemical Society

Bratislava

- Edited by: Jana Shepa, Pavol Jozef Šafárik University in Košice, Institute of Chemistry, Moyzesova 11, 040 01 Košice, Slovakia, jana.hovancova@student.upjs.sk
 Ivana Šišoláková, Pavol Jozef Šafárik University in Košice, Institute of Chemistry, Moyzesova 11, 040 01 Košice, Slovakia, ivana.sisolakova@upjs.sk
- Reviewed by: Renáta Oriňaková, Pavol Jozef Šafárik University in Košice, Institute of Chemistry, Moyzesova 11, 040 01 Košice, Slovakia, renata.orinakova@upjs.sk
 Andrea Straková Fedorková, Pavol Jozef Šafárik University in Košice, Institute of Chemistry, Moyzesova 11, 040 01 Košice, Slovakia, andrea.fedorkova@upjs.sk

Scientifiic Committee:

Assoc. Prof. Andrea Straková Fedorková, UPJŠ Košice Prof. Renáta Oriňaková, UPJŠ Košice Prof. Andrej Oriňak, UPJŠ Košice Dr. Zuzana Orságová Králová, UPJŠ Košice Dr. Ivana Šišoláková, UPJŠ Košice

Organisation Committee:

RNDr. Zuzana Orságová Králová, PhD. RNDr. Ivana Šišoláková, PhD. RNDr. Radka Gorejová RNDr. Jana Shepa Ing. Michaela Halinkovičová RNDr. Andrea Morovská Turoňová, PhD.

This text is licensed under a CC BY-NC-ND 4.0 licence (CC Attribution-NonCommercial-NoDerivatives 4.0)



Available at: https://unibook.upjs.sk Publication date: 19.11.2020

ISBN 978-80-8152-941-2

LIST OF CONTENTS

Preface
First principles perspective on nanostructures in catalysis: K. Honkala7
Two-dimensional nanomaterials: research and applications: M. Omastová, M. Mičušík, N. Bugárová, Y. Soyka, A. Aniskevich, D. Zeleniakiene
On the use of the ICA technique for EV-battery SOH estimation: D-I. Stroe, A. Gismero, E. Schaltz10
Nonenzymatic sensor for determination of glucose modified by gold nanoparticles: V. Niščáková, J. Shepa, R. Oriňaková
NiAg nanocavity films for SERS detection of organic dyes: O. Petruš, J. Macko, R. Oriňaková, V. Socha16
New approach to TiO ₂ based glucose sensors: J.Shepa, I. Šišoláková, R. Oriňaková18
Electrochemical determination of insulin on nanomodified screen printed carbon electrodes: I. Šišoláková, J. Shepa, F. Chovancová, R. Oriňaková
Surface morphology of the compacted metallic materials after immersion in simulated body fluids: R. Gorejová, Z. Orságová Králová, R. Oriňaková, R. Macko, A. Oriňak
Corrosion characteristics of heterogeneous materials composed of metal and metal oxide: M. Kupková, M. Kupka
Fe-based biodegradable implant material cytotoxicity: J. Macko, R. Gorejová, Z. Orságová-Králová, V. Huntošová, R. Oriňaková
Mechanical properties and degradation performance of biodegradable Fe-based materials containing MgO and ZnO nanoparticles: Andrea Morovská Turoňová, Miriam Kupková, Miroslav Džupon, Monika Hrubovčáková.28
Study of nanocrystalline hydroxyapatite coatings electrochemically deposited on titanium implant material: Z. Orságová Králová, R. Gorejová, R. Oriňaková, M. Schnitzer, R. Hudák, M. Kozák, T. Sopčák, K. Kovaľ, A. Oriňak
Influence of polymeric coating on corrosion properties of iron-based biodegradable materials: M. Petráková, R. Oriňaková, R. Gorejová, A. Oriňak
In particular, research on an encapsulated drug carrier using alginate acid as an outer shell coating: Encapsulation research of ultrafine particles using PEGylated alginate acid and its application. Development and research of drug-encapsulated PEGylated alginate carrier: K. Yagi, A. Oriňak
Corrosion processes in Li-accumulator systems with non-aqueous electrolytes: R. Apostolova, E. Shembel37
Electrochemical performance of specific composites as electrodes for supercapacitors: L. Q. Bao, H. Fei, N. Bugarova, M. Omastova, N. E. Kazantseva, P. Saha
Carbonized MIL-101(Fe)-NH2 as sulphur host for Li-S battery: D. Capková, T. Kazda, M. Almáši, N. Király, A. Straková Fedorková
Cathode material based on sulfur-MWCNTs-PPy-nanopipes for Li-S batteries: K. Gavalierová, A. Straková Fedorková, D. Rueda, P. Gómez-Romero47
Carbon fibers modified with cobalt phosphide nanoparticles as efficient electrocatalysts for hydrogen evolution: A. Gubóová, R. Oriňaková, M. Strečková, J. Shepa
Electrode materials for post-lithium ion batteries based on advanced carbon structures: T. Kazda, D. Škoda51
RuO ₂ -(IrO ₂) films for silicon-based photoelectrochemical water splitting: P. P. Sahoo, M. Mikolášek, K. Hušeková, E. Dobročka, J. Šoltýs, V. Řeháček, L. Harmatha, K. Fröhlich
Influence of oxide nanoparticles on gel polymer electrolyte based on tetraethyl Ammonium tetrafluoroborate: I. Veselkova, M. Sedlaříková
Atomic layer deposition: basic principles and preparation of thin films for energy applications: K. Fröhlich60
Preparation and characterization of the screen printed carbon electrodes modified by zinc nanoparticles for electrochemical insulin determination: F.Chovancová, I. Šišoláková, J. Shepa, R. Oriňaková

Electrochemical enzymatic glucose sensors with immobilized glucose oxidase: D. Kondrakhova, V. Latyshev V. Tomečková, V. Komanický	,
Fabrication of combinatorial materials libraries by flow cell electrodeposition technique: V. Latyshev, S. Vorobiov, O. Shylenko, V. Komanicky)
Investigation of changes in AsxSe100-x amorphous thin films after irradiation with visible light and electron beam: O. Shylenko, B. Bilanych, V. Komanicky	
Numerical model of multiphase catalytic reactions: M. Mačák, P. Vyroubal, J. Maxa	
Catalytic pyrolysis of cellulose catalysed by nanoporous ZnO and ZnO-CuO nanoparticles: N. Podrojková, J. Patera, A. Oriňak, R. Oriňaková	
DFT calculations of CO ₂ activation and conversion on CuO surfaces during heterogeneous catalytic hydrogenation of CO ₂ : N. Podrojková, E. Szlapa, K. Honkala, R. Oriňaková	,
Thermal decomposition of methane using Pd as a catalyst - Theoretical study: K. Sisáková, E. Szlapa, K. Honkala, R. Oriňaková	-
Liquid organic hydrogen carriers (LOHC): K. Sisáková, A. Oriňak, R. Oriňaková)
Modelling of gamma-valerolactone conversion to hydrocarbons over the metallic surface: E. N. Szlapa, M. M. Kauppinen, K. Honkala)

Two-dimensional nanomaterials: research and applications

M. Omastová^{a,*}, M. Mičušík^a, N. Bugárová^a, Y. Soyka^a, A. Aniskevich^b, D. Zeleniakiene^c

^a Polymer Institute SAS, Dubravska cesta 9, 845 41 Bratislava, Slovakia ^b Institute for Mechanics of Materials, University of Latvia, Jelgavas Str. 3, Riga, LV-1004, Latvia ^c Department of Mechanical Engineering, Kaunas University of Technology, Studentu Str. 56, 51424, Kaunas, Lithuania *maria.omastova@savba.sk

The discovery of graphene [1] motivated the scientific community to prepare and study other new two-dimensional (2D) materials. The current intense interest about 2D materials is due to their unique properties resulting from their structure. They offer highly specific surface area as well as electronic structures that can achieve new interesting properties. Graphene and/or graphene oxide particles are intensively studied as promising candidates for various applications as materials for energy storage, photovoltaics, electrical and optical sensors, etc. Graphene based biosensors, including modified graphene oxide (GO) particles are intensively studied nowadays. In particular, the hydrophilic character of GO permits the manufacture of reliable, highly sensitive and ultrafast biosensing nanoplatforms.

MXenes are a new class of 2D inorganic materials, discovered by Barsoum and his group in 2011 [2]. MXenes are prepared from MAX phases of the formula $M_{n+1}AXn$, where M is the most common transition metal, A is an element of the 13 or 14 group of the periodic table, and X is usually C and/or N. By etching of the A layers from MAX phase, MXene are formed. The process of etching caused that surface of MXenes contains functional groups e.g., -O, -F, -OH, and hydrophilicity of these 2D particles.

In this work modification of GO and MXene was studied, and application examples of these 2D fillers will be demonstrated.

A new type of graphene-oxide multifunctional nanoplatform was prepared for the detection of tumor cells. In a first step, GO nanolayers were prepared and functionalized with magnetic nanoparticles and a monoclonal antibody (MAb) specific for CA IX cancer marker. Prepared GO platforms were characterized in terms of oxidation, nanoparticle size and exfoliation, using various physical and chemical methods. Magnetic nanoparticles (MNps) were prepared by the chemical precipitation method and their surface was modified by poly-L-lysine. CA IX-specific antibody was attached via an amide bond to a modified magnetic nanoparticle that was conjugated to the GO platform again via an amide bond. After performing toxicological tests on a cell line, no effect of the cytotoxicity of the multifunctional GO platforms was found. The selectivity of GO-MNps-MAb platforms to target tumor cells has been demonstrated. The results also provided promising evidence of tumor cell targeting with a wide potential for visualization and future tumor treatment [3].

 $Ti_3C_2T_z$ MXenes were prepared by the hydrochloric acid/lithium fluoride etching of MAX phase type Ti_3AlC_2 . The characterisation of MXenes, and MXene coatings was carried out with XPS, AFM, and SEM analyses [4]. The stability of MXene layers was study within few months by conductivity measurement.

Experimental condition of MAX phase etching and methods of MXene preparation significantly influence the final electrical conductivity of MXenes [5]. It is found that the high electrical conductivity and mobility of MXene can accelerate the charge transfer, what opened opportunities for the use of MXene as potential materials solar cell applications, in batteries and supercapacitors.

Acknowledgements

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 777810, and by project APVV 14-0120 (Slovakia).

References

[1] K.S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, Y. Zhang, S.V. Dubonos, I.V. Grigorieva, A.A. Firsov. Science. 306 (2004) 666-669.

[2] M. Naguib, M. Kurtoglu, V. Presser, J. Lu, J. Niu, M. Heon, L. Hultman, Y. Gogotsi, M. W. Barsoum. Adv. Materials, 23 (2011) 4248-4253.

[3] N. Bugárová, Z. Špitálsky, M. Mičušík, M. Bodík, P. Šiffalovič, M. Koneracká, V. Závišová, M. Omastová, et.al. Cancers, 11 (2019) art. no. 753.

[4] V. Gajdošová. L. Lorencová, M. Procházka, M. Mičušík, M. Omastová, S. Procházková, F. Kvetoň, M. Jerigová, D. Velič, P. Kasák, J. Tkáč. Microchimica Acta. 187, (2020) art. no. 52.

[5] K. Zukiene, G. Monastyreckis, S. Kilikevicius, M. Prochazka, Micusik, M. Omastova, A. Aniskevich, D. Zeleniakiene. Mat. Chem. Phys. 257 (2021) 123820.