PHYSICAL CHEMISTRY 2021

4th International Meeting
on

Materials Science for Energy Related Applications

BOOK OF ABSTRACTS

September 22-23, 2021
University of Belgrade - Faculty of Physical Chemistry, Belgrade

UNIVERSITY OF BELGRADE
FACULTY OF PHYSICAL CHEMISTRY
Belgrade, Serbia

THE SOCIETY OF
PHYSICAL CHEMISTS OF SERBIA
Belgrade, Serbia

4th International Meeting

on

Materials Science for Energy Related Applications

held on September 22-23, 2021 at the

University of Belgrade, Faculty of Physical Chemistry,

Belgrade, Serbia

(online meeting)

is a satellite event of

PHYSICAL CHEMISTRY 2021

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FACULTY OF PHYSICAL CHEMISTRY
Belgrade, Serbia

in co-operation with

THE SOCIETY OF PHYSICAL CHEMISTS OF SERBIA

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Editors

Prof. Dr. Igor A. Pašti

Assist. Prof. Dr. Ana S. Dobrota

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Preface

International Meeting on Materials Science for Energy-Related Application (IMMSERA) was launched in 2014 as a satellite event of the Physical Chemistry conference series. It is a biannual event, but Covid-19 pandemics resulted in a three-year gap as the last meeting took place in 2018.

For that reason, 4IMMSERA is a completely online event. We are happy that IMMSERA is taking place but aware that an online event cannot replace real on-site knowledge sharing as discussion. Therefore, we present two plenary lectures (Prof. Coy and Dr. Smiljanic) and 35 oral presentations divided into six sessions this year. We hope that the exchange of knowledge and new findings and discussion will be productive in this difficult situation.

Looking back at the development of IMMSERA, we believe that the meeting has reached a critical mass and that it requires rebranding. The next meeting, 5IMMSERA, will grow to a stand-alone event with a pre-tailored programme covering state-of-the-art developments in the field of energy-related materials, with approximately 50% of invited lectures. We shall retain a small format of the meeting – within 2 days we aim to approximately 40 oral presentations, without any overlap between conference sessions, allowing every participant to participate in the discussion of presented results. We strive for scientific excellence and the formation of a hotspot to exchange scientific ideas and top-level scientific results.

We thank all the participants of 4IMMSERA and hope that the dissemination of their research will bring new ideas and collaborations.

Editors

Prof. Dr. Igor Pašti,

University of Belgrade – Faculty of Physical Chemistry

Dr. Ana S. Dobrota, assistant professor,

University of Belgrade – Faculty of Physical Chemistry

T A B L E O F C O N T E N T

Session 1 – Materials for electrochemical power sources

Session 4 – Catalysis, electrocatalysis and photocatalysis in energy conversion and storage

Session 5 – First Steps in Materials Science - Student's Pitch presentation section

Session 6 - General

MODIFICATION OF SURFACE OXYGEN GROUPS OF GRAPHENE OXIDE BY ION BEAM IRRADIATION FOR SUPERCAPACITOR APPLICATIONS

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Surface oxygen groups may have a significant impact on the electrochemical charge storage properties of graphene oxide (GO). The presence of these groups on GO should be properly balanced so that electronic conductivity is optimized, while only the groups that are beneficial to capacitance are preserved. Ion beam irradiation can be identified as a technique where a controllable change of surface chemistry and structure of GO is possible through varying the energy and the fluence of an ion beam. In the present study, the influence of proton-beam irradiation on the surface chemistry and structural properties of GO paper was investigated. GO paper was irradiated with 15 keV proton-beam to fluences from 5×10^{16} to 2×10^{17} ions cm^{-2}, while Fourier-transform infrared spectroscopy (ATR-FTIR), X-ray photoelectron spectroscopy (XPS), and Raman spectroscopy (RS) were used for the analysis of the surface chemistry and structural properties. Results indicate increasing reduction of surface oxygen groups and the preferential removal of the alkoxy and epoxy groups as fluence increased. Desorption of these basal plane groups was outlined in our previous work as important for charge storage capacity, probably due to conductivity increase [1]. When oxygen content was compared to: 1) relative areas of specific functional groups from FTIR and XPS and 2) parameters of Raman peaks, an interesting correlation was found that suggest optimal fluences for tuning the surface chemistry and structural properties of GO. Modification of surface chemistry originates from the physical and chemical effects of ion beam irradiation which were also investigated theoretically. The interaction of functional groups with H-atom was investigated using DFT and semi-empirical (SE) approach. SE calculations revealed that the chemical reduction of the epoxy group appears at H-atom energies below 1.5 eV. Results indicate that ion-beam irradiation can be used for controllable modification of surface chemistry of GO where the applied fluence can be used for tuning the degree of change, which may have implications to electrochemical charge storage properties.

References:

[1] Z. Jovanović *et al.*, Electrochim. Acta, **258** (2017) 1228-1243.