

The Serbian Society for Ceramic Materials
Institute for Multidisciplinary Research (IMSI), University of Belgrade
Institute of Physics, University of Belgrade
Center of Excellence for the Synthesis, Processing and Characterization of
Materials for use in Extreme Conditions "CEXTREME LAB" - Institute of
Nuclear Sciences "Vinča", University of Belgrade
Faculty of Mechanical Engineering, University of Belgrade
Center for Green Technologies, Institute for Multidisciplinary Research,
University of Belgrade
Faculty of Technology and Metallurgy, University of Belgrade
Faculty of Technology, University of Novi Sad

A microscopic image of ceramic particles, showing a transition from white to red. The particles are spherical and densely packed. The top half is white, and the bottom half is red, with a horizontal boundary line.

PROGRAMME and the BOOK of ABSTRACTS

5CSCS-2019

5th Conference of
the Serbian Society for Ceramic Materials
June 11-13.2019. Belgrade Serbia

Edited by:
Branko Matović
Zorica Branković
Aleksandra Dapčević
Vladimir V. Srdić

Programme and Book of Abstracts of The Fifth Conference of The Serbian Society for Ceramic Materilas **publishes abstracts from the field of ceramics, which are presented at international Conference.**

Editors-in-Chief

Dr. Branko Matović

Dr. Zorica Branković

Prof. Aleksandra Dapčević

Prof. Vladimir V. Srdić

Publisher

Institute for Multidisciplinary Research, University of Belgrade

Kneza Višeslava 1, 11000 Belgrade, Serbia

For Publisher

Prof. Dr Sonja Veljović Jovanović

Printing layout

Vladimir V. Srdić

Press

Faculty of Technology and Metallurgy, Research and Development Centre of Printing Technology, Karnegijeva 4, Belgrade, Serbia

Published: 2019

Circulation: 150 copies

CIP - Каталогизacija у публикацији - Народна библиотека Србије, Београд

666.3/.7(048)

66.017/.018(048)

DRUŠTVO za keramičke materijale Srbije. Konferencija (5 ; 2019 ; Beograd)

Programme ; and the Book of Abstracts / 5th Conference of The Serbian Society for Ceramic Materials, 5CSCS-2019, June 11-13, 2019, Belgrade, Serbia ; [organizers]

The Serbian Society for Ceramic Materials ... [et al.] ; edited by Branko Matović ...

[et al.]. - Belgrade : Institute for Multidisciplinary Research, University, 2019

(Beograd : Faculty of Technology and Metallurgy, Research and Development Centre of Printing Technology). - 139 str. : ilustr. ; 24 cm

Tiraž 150. - Str. 6: Welcome message / Branko Matovic. - Registar.

ISBN 978-86-80109-22-0

a) Керамика - Апстракти

b) Наука о материјалима - Апстракти

c) Наноматеријали - Апстракти

COBISS.SR-ID 276897292

The Serbian Society for Ceramic Materials
Institute for Multidisciplinary Research (IMSI), University of Belgrade
Institute of Physics, University of Belgrade
Center of Excellence for the Synthesis, Processing and Characterization of
Materials for use in Extreme Conditions “CEXTREME LAB” -
Institute of Nuclear Sciences “Vinča”, University of Belgrade
Faculty of Mechanical Engineering, University of Belgrade
Center for Green Technologies, Institute for Multidisciplinary Research,
University of Belgrade
Faculty of Technology and Metallurgy, University of Belgrade
Faculty of Technology, University of Novi Sad

PROGRAMME AND THE BOOK OF ABSTRACTS

**5th Conference of The Serbian Society for
Ceramic Materials**

June 11-13, 2019
Belgrade, Serbia
5CSCS-2019

Edited by:
Branko Matović
Zorica Branković
Aleksandra Dapčević
Vladimir V. Srdić

O-4

FIRST-PRINCIPLES INVESTIGATIONS OF ZnO/ZnS MIXED COMPOUNDS, POLYTYPISM AND (HETERO)STRUCTURES

Dejan Zagorac^{1,2}, Jelena Zagorac^{1,2}, Tamara Škundrić^{1,3},
Dušica Jovanović^{1,3}, Maria Čebela¹, Dragana Jordanov¹, Milena Rosić¹,
Branko Matović^{1,2}

¹*Materials Science Laboratory, Institute of Nuclear Sciences “Vinča”,
University of Belgrade, Serbia*

²*Center for Synthesis, Processing and Characterization of Materials for
Application in the Extreme Conditions “CextremeLab”, Belgrade, Serbia*

³*Dept. Chemistry, Faculty of Sciences & Mathematics, University of Niš, Serbia*

Zinc oxide (ZnO) is one of the most extensively investigated compounds in computational and experimental materials science, but in nature it only rarely occurs in pure form, as the mineral zincite. In contrast, zinc sulfide (ZnS) is very common and the main source of zinc found in nature, where it mainly appears as the mineral sphalerite. Both compounds have a large number of desirable properties for industrial applications, where they are successfully employed in electronics (e.g. LED, LCD, etc.), batteries and in optical materials, as well as additives to various materials, closely related to the structure–property relationships. As ZnS is the most common natural form of zinc, whereas ZnO is rarely found, it is not surprising that ZnO/ZnS solid solutions have not been found in nature. Recently, studies of ZnO/ZnS heterostructures and heterojunctions with various morphologies have been reported usually presenting improved physical and chemical properties for biosensors, electronics, magnetism, optics, catalysis, mechanics and electrochemistry. The main topic of this study are newly discovered ZnO/ZnS polytypes, which provide alternative structural arrangements of ZnO/ZnS compounds, including bulk crystal structures, various nanostructures, heterostructures and heterojunctions. In particular, pristine ZnO and ZnS compounds and mixed ZnO_{1-x}S_x compounds (x = 0.20, 0.25, 0.33, 0.50, 0.60, 0.66, and 0.75) have been investigated. First-principles calculations have been performed using Density Functional Theory (DFT), Local Density Approximation (LDA) and hybrid Heyd–Scuseria–Ernzerhof (HSE06) functionals. A multitude of possible stable polytypes for ZnO/ZnS compounds have been discovered creating new possibilities for synthesis of new materials with improved physical and chemical properties.

1. D. Zagorac, J. Zagorac, J.C. Schön, N. Stojanović, B. Matović, *Acta Cryst. B*, **74** (2018) 628.