

The Serbian Society for Ceramic Materials
Institute for Multidisciplinary Research, 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

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 line separating the two colors.

PROGRAMME and the BOOK of ABSTRACTS

4CSCS-2017

4th Conference of
the Serbian Society for Ceramic Materials
June 14-16.2017. Belgrade Serbia

Edited by:
Branko Matović
Zorica Branković
Dušan Bućevac
Vladimir V. Srdić

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Editors-in-Chief

Dr Branko Matović
Dr. Zorica Branković
Dr. Dušan Bučevac
Prof. Vladimir V. Srdić

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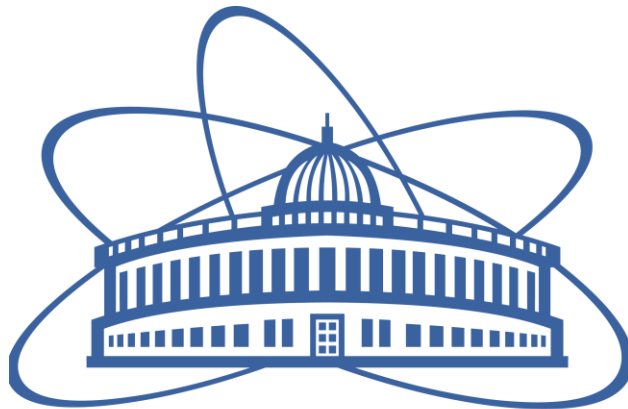
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SPECIAL THANKS TO



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P-9

BiFeO₃ PEROVSKITES: THEORETICAL AND EXPERIMENTAL INVESTIGATIONS

Maria Čebela¹, Dejan Zagorac¹, Jelena Zagorac¹, Radmila Hercigonja²,
Branko Matović¹

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

²*Faculty of Physical Chemistry, University of Belgrade, Serbia*

Bismuth ferrite (BiFeO₃) is one of the most studied multiferroic system. BiFeO₃ has been synthesized by controlled hydrothermal process, where the particles of small sizes and with high purity were obtained. Structural analysis showed that non-annealed powder can be perfectly fitted to rhombohedral space group *R3c* as α -BiFeO₃ phase. In addition, a structure prediction has been performed and 11 additional BiFeO₃ modifications have been proposed. In the next phase, an *ab initio* optimization of predicted structures has been performed and the structure of the γ -phase has been elucidated.

In addition, electronic and magnetic properties of BiFeO₃ were investigated using combination of experimental and theoretical methods. Theoretical studies were performed using a full potential linearized augmented plane-waves plus local orbital (FP(L)APW+lo) method, based on density functional theory (DFT). HRTEM analysis confirmed existence of twin stacking faults, which are responsible for enhanced magnetic properties. EPR measurements suggested existence of electrons trapped by vacancies or defects, while magnetic behavior of synthesized material was investigated by SQUID.