

## Serbian Ceramic Society Conference ADVANCED CERAMICS AND APPLICATION V New Frontiers in Multifunctional Material Science and Processing

Serbian Ceramic Society Institute of Technical Sciences of SASA Institute for Testing of Materials Institute of Chemistry Technology and Metallurgy Institute for Technology of Nuclear and Other Raw Mineral Materials School of Electrical Engineering and Computer Science of Applied Studies

# **PROGRAM AND THE BOOK OF ABSTRACTS**

Serbian Academy of Sciences and Arts, Knez Mihailova 35 Serbia, Belgrade, 21st-23rd September 2016.

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Serbian Academy of Sciences and Arts, Knez Mihailova 35 Serbia, Belgrade, 21-23. September 2016. (MOS). Furthermore, the properties of these components used as switches will be analysed from the power consumption in stable states; switching times; and influence of parasitics point of view, for the first time. To achieve as realistic simulation results as possible the (SPICE) transistor models used here were obtained from the component producers.

#### OR3

#### The nonorthogonality effects on capacitive behaviour of quantum dot

<u>Miloš S. Dražić</u>, Ivana Đurišić, Viktor Z. Cerovski and Radomir Žikić Institute of Physics, University of Belgrade, Pregrevica 118, Belgrade

It is known that the overlap between atomic orbitals produce nontrivial effects on chemical bonds strength, resonance molecular energies, sensitivity of bond orders and charge densities in hetero-molecules. It is also strongly involved in population analysis problem. In quantum transport through a molecule/quantum dot attached between two electrodes, numerical codes rely on some predefined nonorthogonal basis sets. In steady state transport nonorthogonality has no influence on final results for transmission or current. The situation significantly changes when we have to deal with time dependent transport where charge starts to pile up in central region consisting of a molecule with additional neighboring parts of electrodes, chosen in such a way to provides complete screening of a molecule. The nonorthogonality introduces a problem due to nonunique definition of time dependent partial charges associated with electrodes and central region, which is a consequence of nonorthogonality between complementary subspaces, making the corresponding projectors non-Hermitian. The problem is solved in nonequilibrium Green's functions formalism within linear response theory and the derived current expression clearly indicates that the occurrences of additional contributions on interfaces, compared with orthogonal description, can be associated with the displacement current. In a simple comparative analysis it is demonstrated that there is a frequency range around resonances where capacitive response is only due to nonorthogonality.

#### OR4

#### Spectroscopy Characterization of YFeO<sub>3</sub> Obtained by the Mechanochemically Synthesis

Zorica Ž. Lazarević<sup>1</sup>, Čedomir Jovalekić<sup>2</sup>, Dalibor Sekulić<sup>3</sup>, Valentin N. Ivanovski<sup>4</sup>,

Ana Umićević<sup>4</sup>, Martina Gilić<sup>1</sup>, Nebojša Ž. Romčević<sup>1</sup> <sup>1</sup>Institute of Physics, University of Belgrade, Pregrevica 118, Zemun, Belgrade, Serbia <sup>2</sup>The Institute for Multidisciplinary Research, University of Belgrade, Belgrade, Serbia <sup>3</sup>Faculty of Technical Sciences, University of Novi Sad, Novi Sad, Serbia <sup>4</sup>Institute of Nuclear Sciences Vinča, University of Belgrade, Belgrade, Serbia

In the past few years, a renewed interest has grown in the study of rare-earth orthorhombic perovskites. An important example of this trend is the family of rare-earth orthoferrites, which a general formula  $RFeO_3$ , where *R* is the trivalent rare-earth metal ion. YFeO<sub>3</sub> has been prepared by a mechanochemical synthesis in a planetary ball mill. The mechanochemical reaction leading to formation of the YFeO<sub>3</sub> phase was followed by X-ray diffraction, Raman and infr-

arad spectroscopy. The ortoferrite phase formation was first observed after 1 h of milling and its formation was completed after 2.5 h. The synthesized YFeO<sub>3</sub> ferrite has a nanocrystalline structure with a crystallite size of about 12.4 nm. There are five Raman active modes. <sup>57</sup>Fe Mössbauer spectroscopy was performed in order to provide information on Fe compounds in the Y<sub>2</sub>O<sub>3</sub> and  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> mixture.

#### OR5 Synthesis and structural characterization of some cathode materials for lithium-ion batteries

<u>Dragana Jugović<sup>1</sup></u> and Miodrag Mitrić<sup>2</sup> <sup>1</sup>Institute of Technical Sciences of SASA, Belgrade, Serbia <sup>2</sup>Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia

Lithium-ion batteries are under intense scrutiny as alternative energy/power sources. Their electrochemistry is based on intercalation/deintercalation reactions of lithium ions within a crystal structure of an electrode material. Therefore, the structure itself determines both the electrode operating voltage and the transport pathways for lithium ions. Some oxide- and polyanion-based materials are synthesized and studied as positive electrodes. Several synthetic routes were investigated. The crystal structure refinement of an X-ray powder diffraction data was based on the Rietveld full profile method. All relevant structural and microstructural crystal parameters that could be significant for electrochemical intercalation/deintercalation processes were determined. Structural analysis revealed different dimensionality of lithium ion motion. It was also shown that the structural and microstructural properties are significantly dependent on the synthesis condition.

#### OR6

#### Application of ceramic components in knee arthroplasties

<u>Aleksandar Radunović</u> MD,MMA,Belgrade, Serbia Popović Zoran MD, PhD, Vožd clinic,Belgrade, Serbia Aleksandar Jevtić MD, MMA, Belgrade ,Serbia

Total knee arthroplasty is considered as very reliable and efficient procedure with excellent good-therm results. Despite significant improvements in endoprosthesis design and materials for their fabrication, debris induced aseptic loosening of the endoprosthesis is, accompanied by the malpositioning of the components, most frequent cause of the need for revision surgery. Beside this problems, there is growing number of reports of metal allergy as possible causer of procedure failure. For above mentioned, ceramics with its properties attracts attention as a material for endoprosthesis manufacturing. After relatively bad results in the early years of use, followed by improvements in materials and design of endoprosthesis, ceramics look like a promising solution, especially for patients with allergies on metal.