Serbian Ceramic Society Conference
ADVANCED CERAMICS AND APPLICATION XI
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

PROGRAM AND THE BOOK OF ABSTRACTS

Serbian Academy of Sciences and Arts, Knez Mihailova 35
Serbia, Belgrade, 18-20. September 2023.

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structural characterization methods (XRD, FTIR, RAMAN) and electrochemical examination of developed materials in Na-containing organic and aqueous electrolytes using Cyclic Voltammetry and Galvanostatic cycling. Key synthesis steps for designing hard carbon surface and polyanionic composition, with a high capability of storing Na ions, will be identified and elaborated. The results will be discussed in terms of strengths &weaknesses of materials as well as next steps towards developing a safe and reliable Na-ion full cell.
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Modeling & Simulation of Advanced Ceramic Materials

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Innovative materials used in high-technology applications are called advanced materials. These materials can be completely new or typical traditional materials (e.g., metals, ceramics)whose properties have been enhanced to become advanced. This talk will cover the theoretical investigation of various advanced ceramic materials in connection to the experimental results. The first part will include the basics of modeling and structure prediction of ceramic materials, such as global optimization, quantum mechanics, and supercell method, as well as current developments in the Inorganic Crystal Structure Database (ICSD), theoretical crystal structure data, and data mining.In the next part, theoretical methods will be applied to the specific ceramic compounds. A plethora of state-of-the-art quantum mechanical methods will be presented, including Density-functional theory (DFT),LDA-PZ and GGA-PBE, or hybrid B3LYP and HSE functionals, and a combination of quantum mechanics with data mining and global optimization, as well as the newly developed Primitive Cell approach for Atom Exchange (PCAE) method applied on ZnO/ZnS polytypic (hetero)structures and unknown Cr_2SiN_4 compounds. Finally, the theoretical modeling of materials properties has been presented. Since many of the investigated materials show a large number of desirable properties for industrial applications,*ab initio* calculations of electronic, elastic, and mechanical properties will be presented and compared with experiments when available.