



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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there existed a critical concentration of Li^+ that accounted for preferential incorporation of Li^+ into MgAl_2O_4 lattice. Transition metal fluorides were also found to promote densification, while acting as a source of optically active dopants. MnF_2 and CoF_2 promoted the densification as effectively as LiF but caused significant grain growth.

INV5

From brookite-based nanopowder towards titanate nanoribbons: structure and application

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TiO_2 nanopowder based on brookite phase was synthesized using sol-gel hydrothermal method. For the purposes of preparing one-dimensional (1D) nanoribbons, the obtained TiO_2 nanopowder was used as a precursor following an alkaline hydrothermal approach, after which an annealing process took place. The aim of the talk is to provide insight into the effect of the nature of brookite-based nanoparticles on the formation of titanate. Besides that, the results will be discussed in terms of correlation of materials photocatalytic activity with morphological and structural properties. The crystal structure of the synthesized nanomaterials was analyzed by X-ray powder diffraction (XRPD). Besides the XRPD pattern, the structural and morphological characteristics of obtained nanopowders and nanoribbons were also investigated by Raman spectroscopy and Field Emission Scanning Electron Microscopy (FESEM). Conventional and high-resolution transmission electron microscopy (TEM/HRTEM), was carried out for further morphological and crystal structure examination. Synthesized nanostructures were tested in photocatalytic degradation of Reactive Orange (RO16) azo-dye, since these dyes represent the most toxic ones among various types of dyes. The TiO_2 brookite-based nanopowders showed the best photocatalytic efficiency, whereas the titanate after annealing were much faster in degradation in comparison with titanate obtained after hydrothermal process.

INV6

DFT Analysis of Hyperfine Couplings in *d* and *f* metal complexes with Tetrahydro Borate Ligands

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Metal complexes with BH_4^- ligands show extravagant structural and dynamic properties, and possess many important and applicable qualities (potent reducing agents and catalysts, materials for hydrogen storage). Electron paramagnetic resonance (EPR) is very important for the characterization of complex compounds, determination of their electronic configuration and geometry. Also, Density Functional Theory (DFT) can predict EPR parameters and

explain them more profoundly. Of particular importance is the analysis and prediction of hyperfine coupling constants for lanthanide complexes with BH_4^- ligands, given that there is not much data in the literature. Within this paper hyperfine coupling constants of d and f metal complexes with BH_4^- ligands have been determined by DFT calculations, and analyzed in detail. Calculations predicted that proton hyperfine coupling constants are very small in the case of complexes of f elements, and are present only due to weak polarization. The increase of covalence and the number of unpaired electrons does not significantly affect the change of constants of BH_4^- ligands, but only of protons that are bound by σ bonds.

INV7

Modelling of stacking interactions relevant to non-metallic electronic materials

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Tetrathiafulvalene (TTF) and tetracyanoquinodimethane (TCNQ) are organic compounds of great importance for the development of non-metallic materials, most notably charge-transfer salts. Parallel packing is very common in crystal structures containing TTF and TCNQ units, and the formation of stacking interactions between these fragments influences the conductivity properties of these materials. The geometries of these stacking interactions were described based on the crystal structures deposited in the Cambridge Structural Database that contain TTF or TCNQ pairs. The calculations of interaction energies between two neutral TTF molecules, as well as between two neutral TCNQ molecules, performed at B2PLYP-D3BJ/6-311++G** and TPSS-D3/def2-TZVP levels of theory, respectively, showed that the geometries of the strongest stacking interactions correspond to the most frequent ones in the crystal structures. The strongest interactions have energies of -9.96 kcal/mol and -8.03 kcal/mol for TTF and TCNQ dimers, respectively, showing the ability of these molecules to form strong stacking interactions. The obtained energies were supported by the SAPT energy decomposition analysis, as well as the electrostatic potential surfaces of isolated monomers, showing the nature of these stacking interactions. The strongest stacking interactions are shown to be the ones that support the high conductivity of TTF and TCNQ-based materials.