

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 of Excellence for Green Technologies, Institute for Multidisciplinary  
Research, University of Belgrade  
Faculty of Technology and Metallurgy, University of Belgrade

# PROGRAMME and the BOOK of ABSTRACTS

6CSCS-2022

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**Branko Matović**  
**Aleksandra Dapčević**  
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P-37

## STRUCTURAL AND MECHANICAL PROPERTIES OF HIGH-ENTROPY ALLOYS (HEAS) - ULTRA-HIGH TEMPERATURE CERAMICS (UHTC) ON DFT LEVEL

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High-Entropy Alloys (HEAs) have attracted considerable interest due to the combination of useful properties and enhanced applications, and a few HEAs have already been shown to possess exceptional properties under extreme conditions (e.g. Ultra-High Temperature Ceramic (UHTC)). However, predicting the formation, structures, and stability of HEAs is one of the major goals of recent studies, which is expected to bring discovery of new systems with enhanced properties of the material, with special attention on high temperature and mechanical load. Here, we show an example of high-entropy rare-earth (RE) zirconates with a pyrochlore structure that was examined theoretically and experimentally observed. Theoretical methods were applied to investigate the variable composition of the ordered and disordered pyrochlore structures using quantum mechanics, group action theory, PCAE, and supercell methods. The investigated RE<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub> compound was successfully fabricated by pressureless and spark plasma sintering. with nominal composition (La<sub>0.2</sub>Y<sub>0.2</sub>Gd<sub>0.2</sub>Nd<sub>0.2</sub>Sm<sub>0.2</sub>)Zr<sub>2</sub>O<sub>7</sub>, prepared by simple glycine nitrate procedure (GNP) and characterized using various experimental methods (XRD, SEM, TEM, Raman, etc.). [1] Pyrochlore structures were generated using the Primitive Cell Approach for Atom Exchange (PCAE) method [2] or the supercell approach using the Crystal17 program package [3], and investigation of disordered systems and solid solutions was conducted using the group action theory [4]. Structural optimization on the *ab initio* level was performed using the Crystal17 code, based on a Linear Combination of Atomic Orbitals (LCAO). Density

functional theory (DFT) calculations were utilized in the present study, using the local density approximation (LDA) with Perdew-Zunger (PZ) correlation functional.

1. B. Matović, D. Zagorac, I. Cvijović-Alagić, J. Zagorac, S. Butulija, J. Erčić, O. Hanzel, R. Sedlák, M. Lisnichuk, P. Tatarko, *Bol. Soc. Española Cerám. V.*, (2021).
2. D. Zagorac, J. Zagorac, J.C. Schön, N. Stojanovic, B. Matovic, *Acta Crystallogr. Sect. B: Struct. Sci. Cryst. Eng. Mater.*, **74** (2018) 628–642.
3. R. Dovesi, F. Pascale, B. Civalleri, K. Doll, N.M. Harrison, I. Bush, P. D'arco, Y. Noël, M. Rérat, P. Carbonniere, *J. Chem. Phys.*, **152** (2020) 204111.
4. S. Mustapha, P. D'Arco, M. De La Pierre, Y. Noël, M. Ferrabone, R. Dovesi, *J. Phys.: Condens. Matter*, **25** (2013) 105401.

P-38

## **PREDICTION OF STRUCTURE CANDIDATES FOR SiB<sub>6</sub> COMPOUND USING A COMBINATION OF DATA MINING AND THE PCAE METHOD**

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Silicon borides represent very appealing industrial materials for research due to their extraordinary features. Discovered at the beginning of the XX century, SiB<sub>6</sub> is considered as one of the most elusive refractory compounds as its crystal structure is yet not fully understood. The first reports suggested a cubic SiB<sub>6</sub>, which was followed by an experimentally observed orthorhombic phase, but later studies determined a cubic SiB<sub>6</sub> as an unstable phase and suggested an additional monoclinic *P21/m* space group. In order to predict possible phases within this system of interest, we have undertaken calculations using the ab initio minimization data mining approach [1,2] combined with the PCAE method [3]. Several promising structure candidates have been found and each of the newly found structure candidates was locally optimized on the DFT level, employing the