

INSTITUTE OF TECHNICAL SCIENCES OF SASA
MATERIALS RESEARCH SOCIETY OF SERBIA

Programme and the Book of Abstracts

**TWENTIETH YOUNG RESEARCHERS' CONFERENCE
MATERIALS SCIENCE AND ENGINEERING**

Belgrade, November 30 – December 2, 2022



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Aim of the Conference

Main aim of the conference is to enable young researchers (post-graduate, master or doctoral student, or a PhD holder younger than 35) working in the field of materials science and engineering, to meet their colleagues and exchange experiences about their research.

Topics

Biomaterials
Environmental science
Materials for high-technology applications
Materials for new generation solar cells
Nanostructured materials
New synthesis and processing methods
Theoretical modelling of materials

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Role of halogen substituents in the design of halogen-containing high-energy materials

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It is known that halogen interactions can be a tool for modifying the potential above the central regions of the molecular surfaces of halogen-substituted high-energy molecules (HEMs), which is directly related to the sensitivity towards detonation of those molecules. Also, it is known that the substitution of hydrogen with halogen in some organic molecules which contain a nitro group can affect the dissociation energy of the C – N bond. In this work the molecules of 1,4- and 2,3-halo substituted 5,8-dinitronaphthalene were studied. Electrostatic potential maps were calculated for each of these molecules using the PBE/PBE/6-311G** level of theory. The WFA-SAS program was used to obtain the maps of electrostatic potential. The dissociation energies of C – N bonds in the mentioned molecules were calculated using the SAPT program. Also, the heats of formation and the Widberg bond order were calculated. The results indicate that the halogens will have a much greater influence on the potentials above the central regions of the molecular surfaces in the case when they are located at positions 2 and 3 in 5,8-dinitronaphthalene. However, halogens in positions 1 and 4 lead to a significant decrease in the dissociation energy of C – N bonds, compared to 2,3-substituted analogues. It is believed that these differences are the results of different characteristics of the halogens, but also their positions in relation to the nitro groups.

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