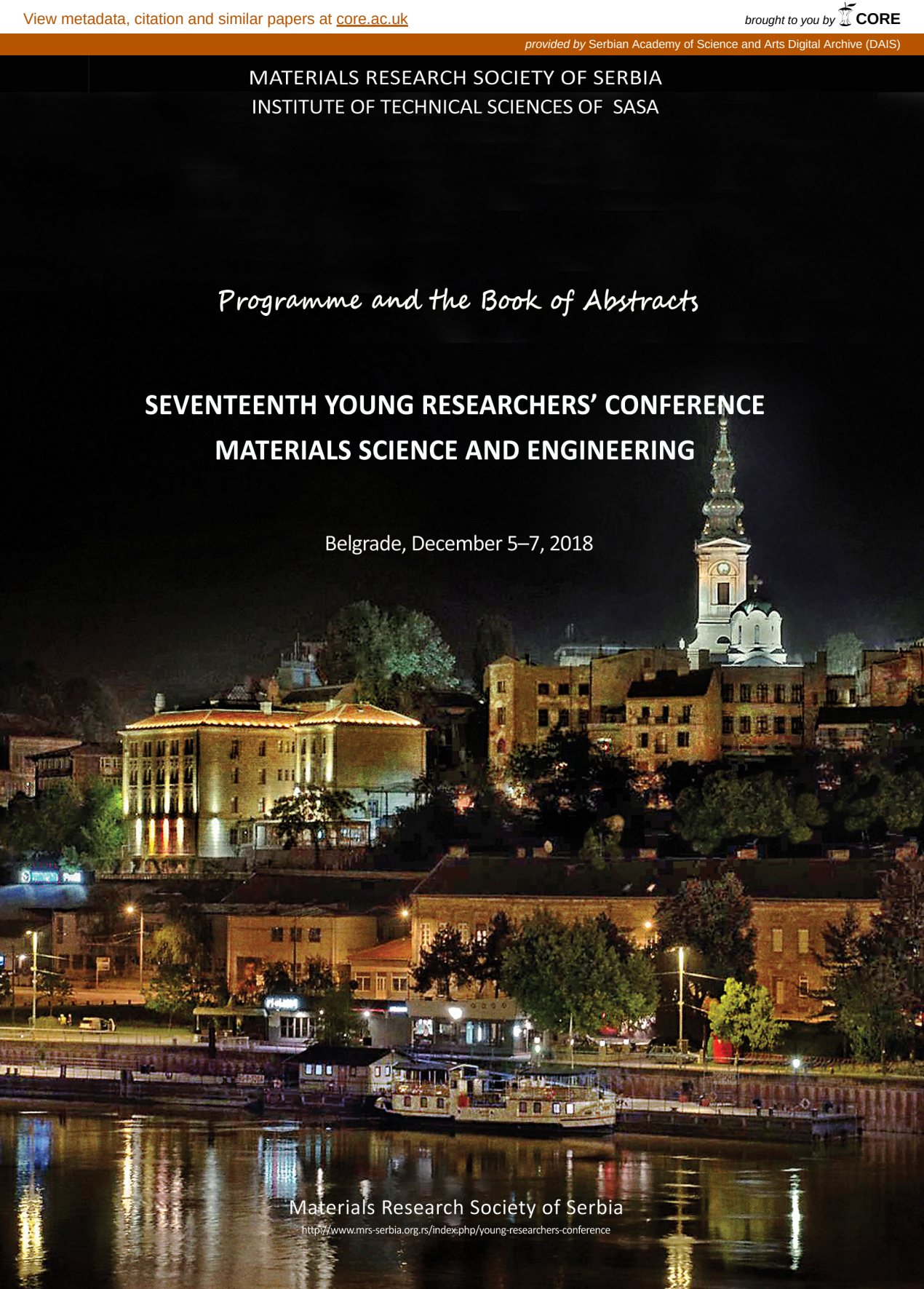
MATERIALS RESEARCH SOCIETY OF SERBIA
INSTITUTE OF TECHNICAL SCIENCES OF SASA

Programme and the Book of Abstracts

SEVENTEENTH YOUNG RESEARCHERS' CONFERENCE MATERIALS SCIENCE AND ENGINEERING

Belgrade, December 5–7, 2018



Materials Research Society of Serbia
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&
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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
Nanostructured materials
New synthesis and processing methods
Theoretical modelling of materials

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Results of the Conference

Beside printed «Program and the Book of Abstracts», which is disseminated to all conference participants, selected and awarded peer-reviewed papers will be published in journal "Tehnika – Novi Materijali". The best presented papers, suggested by Session Chairpersons and selected by Awards Committee, will be proclaimed at the Closing Ceremony. Part of the award is free-of-charge conference fee at YUCOMAT 2019.

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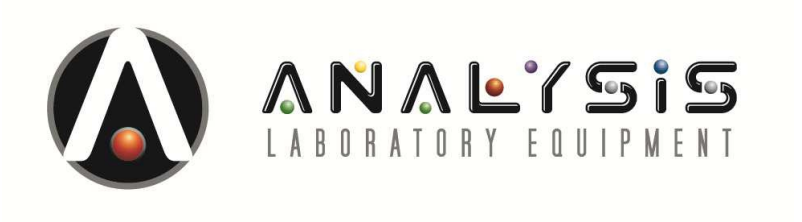

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4-4

Structural properties and antisite defect formation in monoclinic Li_2FeSiO_4 – a DFT aspect

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Properties of monoclinic Li_2FeSiO_4, which is a prominent candidate for future use as a cathode in lithium ion batteries, have been investigated by DFT+U method, using GGA-PBE approximation, plane wave basis set and periodic boundary conditions. All calculations were performed in an antiferromagnetic state, which has been found to be energetically slightly more stable than ferromagnetic. Optimized lattice parameters and atomic coordinates have been compared to the literature data in order to verify the model. In addition, a particular attention was paid to the possibility of the formation of an antisite defect, which was introduced as the interchange between Fe and Li ions at both Li1 and Li2 crystallographic positions. The concentration of defect was varied from 0 to 25 molar per cent. Changes of structural, energetic, and magnetic properties of monoclinic Li_2FeSiO_4 upon increase of Li1-Fe and Li2-Fe antisite defect concentration have been analyzed and discussed in light of available experimental results.