MATERIALS RESEARCH SOCIETY OF SERBIA
INSTITUTE OF TECHNICAL SCIENCES OF SASA

Programme and the Book of Abstracts

EIGHTEENTH YOUNG RESEARCHERS' CONFERENCE
MATERIALS SCIENCE AND ENGINEERING

Belgrade, December 4–6, 2019

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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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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 2020.

Sponsors

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Tuning charge transfer states in the G-octet-metal ion complexes for the potential nanotechnological applications

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At the telomeric, guanine (G) rich region of the DNA, non-canonical biologically relevant nanostructures can be formed including G-quadruplexes. To further improve their stability, binding of the monovalent/bivalent cations is also possible within the G-quadruplex cavity. Due to their unique topological pluralism and self-assembly tendency, they can be used to prepare functional supramolecular assemblies. These structures can be easily integrated in nanodevices. Exploring their excited state properties is of interest for the application in the molecular electronics and optoelectronics. Here we study G-octet-metal ion complexes (M-G_8) which act as models for the G-quadruplex supramolecular arrangement within DNA. We used DFT based molecular dynamics (BLYP-D3/DZVP+PW+GTH) for the configuration sampling purposes and calculated electronic excitations to initially populated (Franck-Condon) states. We use descriptors based on one-electron transition density matrix to seize charge transfer content of the selected excited states. We use TDDFT formalism (CAM-B3LYP/6-31G(d)) to calculate one-electron transition density matrices and absorption spectrum. Results indicate that the M-G_8 (M=Li^+, Na^+, K^+, Mg^{2+}, Ca^{2+}) systems absorption spectrum is slightly modulated by introducing alkali metal ions compared to the empty scaffold. On the other hand, earth-alkali metal ions have somewhat larger impact on the broadness and the red tail of the spectrum. Beside this, charge transfer content is highly modulated and shifted towards lower energies for the Mg^{2+}-G_8 and Ca^{2+}-G_8 systems making them accessible more easily. This feature is not in the correlation with structural arrangement but probably with charge of the templating cation. These results indicate that earth-alkali M-G_8 complexes are more suitable for potential technological applications.