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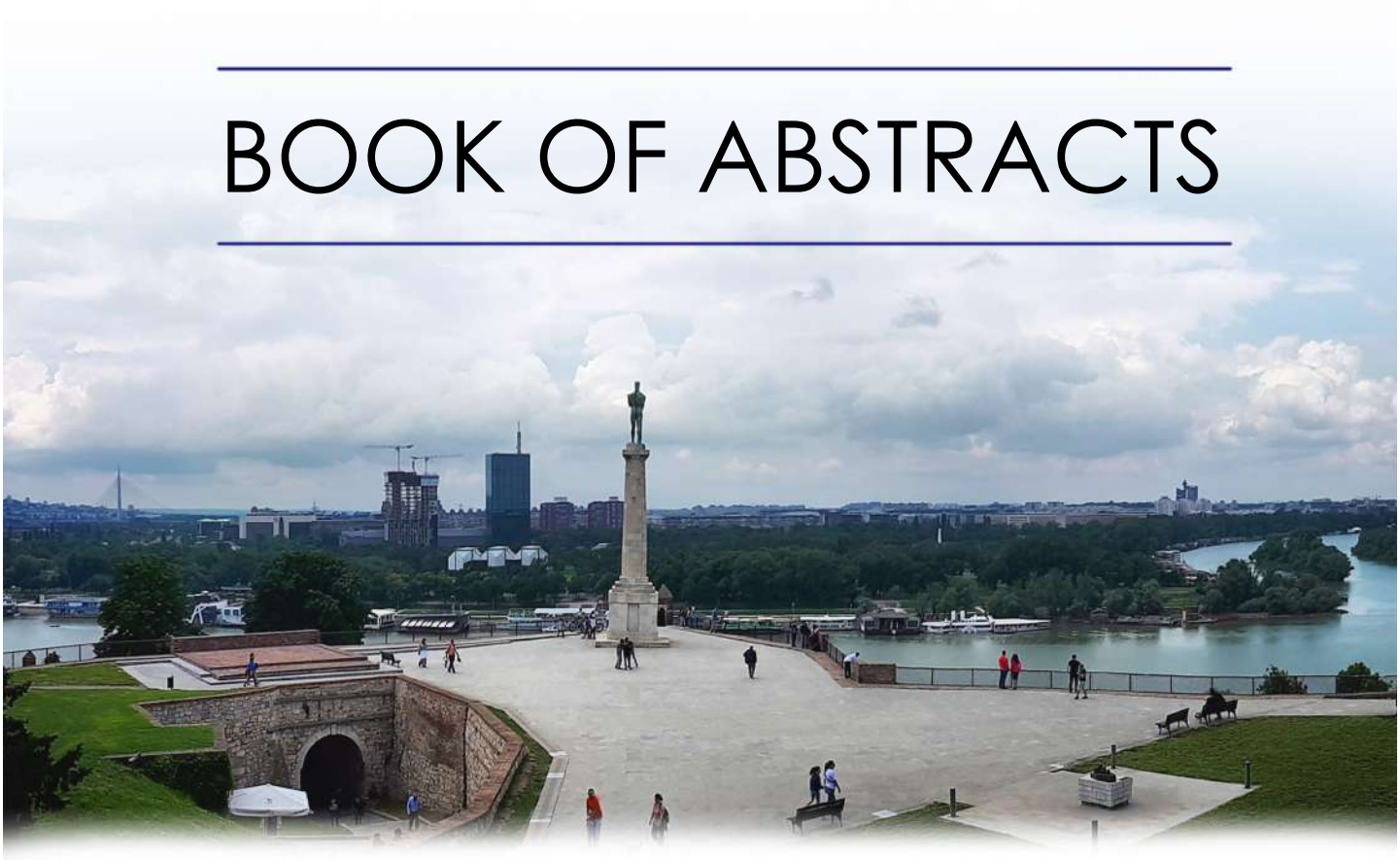
BOOK OF ABSTRACTS



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DNA-Based Dendrimers: Novel Macromolecules With Peculiar Characteristics

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Abstract. We present a joint theoretical-experimental study of a novel class of macromolecules, the so-called dendrimer-like DNAs (DL-DNAs). They have recently been synthesized from the enzymatic ligation of Y-shaped DNA unit, a three-armed structure consisting of double-stranded DNA (ds- DNA), formed via hybridization of three single-stranded DNA chains (ss-DNA), each of which has partially complementary sequences to the other two [1]. To describe such dendrimers of various generations we have employed a bead-spring model, in which base-pairs of a single DL-DNA molecule are modeled by charged monomers, whose interactions are chosen to mimic the equilibrium properties of DNA correctly. We have performed Molecular Dynamics Simulations and we have also employed dynamic/static light scattering in order to determine equillibrium properties and conformational characteristics of all-DNA dendrimers as well as the behavior of their solutions. We have investigated their behavior in ionic solution, paying particular attention on their salt-responsiveness. Our computational and experimental results reveal that the DL-DNAs are rigid objects with low internal monomer concentration, regular voids in their interior, with high persentage of absorbed counterions, and that show high resistance to stimuli-responsiveness [2]. These properties shape the behaviour of their solutions. Namely, both experimental as well as computational results show anomalous structure factor of dense DL-DNA solutions, as it had been predicted theoreticaly in Ref [3]. In this way we have found the object which was a missing puzzle in understanding the full phase diagram of star polymer solutions.

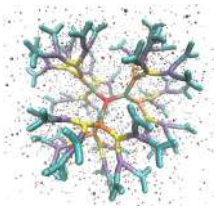

FIGURE 1. 6th generation of the dendrimer composed of Y-shaped DNA building blocks.

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3. Watzlawek, M., Lowen, H., and Likos, C.N., *J. Phys.: Condens. Matter* **10**, 8189-8205 (1998).