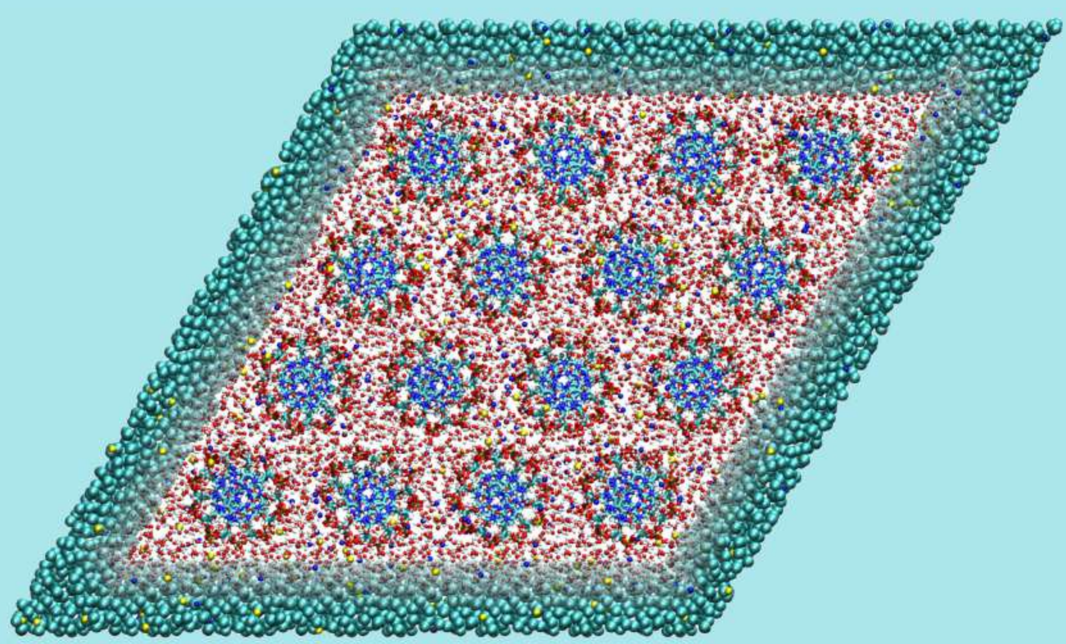
CECAM and IUPAP workshop on

High density DNA arrays: models, theories and multiscale simulations



Book of abstracts

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Contents

DNA-based dendrimers: From a single molecule to the dense solution description

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We present a joint theoretical-experimental study of a novel class of macromolecules, the so-called DNA-based dendrimers. 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]. In order to describe such dendrimers of various generations we have employed two independent models: a bead-spring model and the oxDNA model. In the bead-spring model, 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. On the other hand, the oxDNA model allows us to take a closer look into the DNA structure, treating DNA as a string of rigid nucleotides which interact through potentials that depend on the position and orientation of the nucleotides. 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-DNA 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.

[1] Y. Li, Y. Tseng, and D. Luo, Nat. Mater. **3**, 38, (2004).

[2] C. Jochum, N. Adžić, E. Stiakakis, T. L. Derrien, D. Luo, G. Kahl, and C. N. Likos, Nanoscale, **11**, 1604 (2019).