STRUCTURE OF A CIRCULAR CHAIN CONFINED IN AN ARRAY OF NANOPOSTS

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The function of biomacromolecules in living systems is dictated by their conformation which is considerably modified in geometrically confined or crowded spaces. Thus, knowing the conformation of confined biopolymers is inevitable for understanding the biochemical processes. The single-chain experiments are realized in microfluidic devices. In these experiments, a chain is confined in a rectangular channel of various aspect ratio. The theory of a single linear chain confined in a channel or slit is well elaborated and supported by a great number of simulation studies. A special situation appears when a chain is confined in an array of collinearly organized posts that might be approximated as a system composed of quasi-channels mutually interconnected through a passage between adjacent posts. Nowadays, arrays of nanoposts have been pointed out as very efficient substitutes for gels in electrophoretical devices.[1] This study is focused on the effect of chain stiffness and chain topology on the structural properties of a polymer chain in an array of nanoposts. The structural behavior of a linear flexible and semiflexible (DNA) chain is compared with its circular analogue. Although, the simulations of a linear flexible chain confined in an array of nanoposts have already been reported,[2] the behavior of a circular chain in an array of nanoposts has not been studied yet. Moreover, to the best of our knowledge, the combination of the confinement due to a nanopost array and the chain stiffness on the chain conformation has not been addressed. The number of occupied spaces is evaluated in order to explain the non-monotonic variation of the chain extension with the post diameter. The asymmetry in the chain expansion with respect to the post axes is scrutinized and explained. The system of post arrays is approximated as a combination of a quasi-channel and a quasi-slit like geometry. The interstitial spaces are viewed as being of a channel geometry while the passage between two adjacent posts are viewed as being of a slit geometry. Such an approximation appears to be semi-quantitative. The stiffer chains tend to penetrate more readily into direction perpendicular to the post axes and thus to occupy more interstitial volumes.

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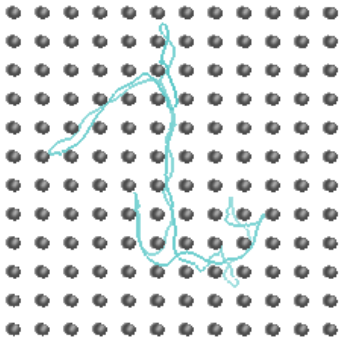

Snapshot of a circular chain in the array of nanoposts, top view.

[1] Volkmuth W. D., Austin R. H. *Nature* **358**, 600-602, 1992.

[2] Joo H., Kim J. S. *Soft Matter* **11**, 8262-8272, 2015.