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Complex Phase Transition of DNA Condensation under Crowding Confinement Conditions

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Abstract

The mechanism underlying the crowding effects that assist the condensation process by multivalent cations under confinement is not yet reported. Based on the strong correlation model, Monte Carlo simulation was implemented to detect the crowding effects on DNA condensation within a capsule-like space, and its geometry controlled by the aspect ratio. With the addition of crowders, the condensed conformations confined within the spherical space (aspect ratio is 1) become more compact than those without crowders. The DNA-condensed conformations undergo a transition from the initial random coil structure to toroid structure, followed by the extended rod-like structure, and finally to totally compacted structure. The critical volume fraction corresponding to the transition from the rod-like structure to totally compacted structure pertained to the crowder size proportionally. Moreover, the critical volume fraction corresponding to the phase transition strongly depends on the confinement geometry, the critical volume fraction for the case with constant radius is inversely proportional to the aspect ratio. Conversely, the case with constant cylinder length showed that the critical volume fraction is proportional to the aspect ratio. These phenomena are consistent with their corresponding phase diagram

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