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Nematic Ordering in Confined Geometry Applied to DNA Packaging in Viral Capsids NIKOLAY OSKOLKOV, Department of Chemistry, University of North Carolina, Chapel Hill, North Carolina 27599-3290, USA, PER LINSE, Department of Physical Chemistry 1, University of Lund, Box 124 SE-221 00 Lund, Sweden, ALEXEI KHOKHLOV, Physics Department, Moscow State University, 119991 Moscow, Russia — We propose a density functional theory of conformation of a double stranded DNA inside a spherical viral capsid. For this purpose we apply the mathematical apparatus elaborated in the classic theories on nematic ordering to describe the arrangement principles of a long persistent polymeric chain in confined geometry. In this way, the local self-assembly of different segments of the chain can be considered as a nematic phase with a non-constant (distorted) director. Taking into account the only steric interactions in the second virial approximation is shown to be enough to demonstrate the principle possibility of the nematic ordering. As a result, the polymer density and orientational order distributions throughout the volume of the capsid were obtained. It is observed that a short and flexible polymeric chain is concentrated at the center of capsid being orientationally disordered, and behaving similar to a simple polymeric coil in the spherical cavity. In contrast, upon the increasing of the length and rigidity of the chain, it shifts towards the surface of the capsid locating predominantly at the equator, and undergoes the nematic transition.

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