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Structural transitions in packing of a semi-flexible chain confined in a sphere ARTEM LEVANDOVSKY, LEONID PRYADKO, ROYA ZANDI, University of California, Riverside — We study phases and phase transitions (crossovers) between phases of a semi-flexible polymer chain confined in a spherical cavity. Such a problem is relevant to DNA or RNA packaging in viruses whose organization is characterized by both simplicity and economy. The confinement involves both energetic and entropic effects controlled by the stiffness of the chain, its length and diameter, and the sphere radius. Formation of different packing configurations and structural changes in these configurations is studied with a non-local “cluster” Monte Carlo method. We introduce several order parameters characterizing different packing symmetries and compute the corresponding probability distributions. This allows us to reconstruct the Landau free energies for these order parameters, and thus develop a simple theory of packing transitions.

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