MACS SG8/SG9 Joint Seminar

Alignment of rods at intra-chain and inter-chain level: Modeling and simulation

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Venue: Seminar room, 2nd Floor
Institute for Advanced Study (KUIAS)
Main Building (#77 on map)

Abstract:

The recent AFM (atomic force microscopy) measurement on the conformation of a single circular DNA in the presence of charged polyamines showed unique compact structures. These structures take up various shapes, such as Y-shaped and linear bundles, etc. To elucidate these structures, we resort to Monte Carlo simulation to investigate a two-dimensional circular semiflexible spring-chain model that mimic locally rigid circular DNA. The monomers, modeled as hard disks, consist of non-interacting and interacting sites. Among interacting monomers, an attractive Yukawa potential is used to depict the corresponding interaction potential in the simulation. The experimental DNA conformations are qualitatively reproducible through fine-tuning chain rigidity and the magnitude of attraction. The Y-shaped and linear bundles can be achieved while interacting/non-interacting monomers are distributed like an alternating copolymer around the ring polymer. Meanwhile, the alignment among intra-chain segments is essential to develop these compact structures. Our simulation provides novel insights into the likely spatial distribution of bound polyamines on DNA. In the second part of this talk, I will briefly discuss about the orientation ordering of rigid rods in a confined cavity under molecular crowding. For long enough rods, they tend to align in the cavity, and the alignment is enhanced by increasing the number of crowders. For shorter rods, the orientation ordering among rods diminishes regardless of crowding levels. A simple picture by considering that the single-layer rods undergo hexagonal packing within a spherical cavity can help us understand the origin of the orientation ordering among confined rods.

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