
Environmental control of stochastic cargo transport by teams of molecular motors

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Abstract

Cargos transported along microtubules are often transported by opposite teams of molecular motors. Based on our simulation results, we show that this feature allows an easy control of the cargo-motors complex dynamics, through the tuning of a single external parameter. Several surprising features are predicted. For example, the complex can speed up when the viscosity is increased. These predictions could be tested in vitro.

*Speaker

A change in stripes for cholesteric shells via modulated anchoring

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Abstract

Chirality, ubiquitous in biological systems from the genetic code to organismic structure, can be controlled and quantified in materials. Indeed, many of the chiral structures found in biological systems are also found in cholesteric liquid crystal (CLC) systems, which can be manipulated through chemistry, geometry, and external fields. In this work, we study spherical shells of CLC made with microfluidics and control the molecular anchoring at the inner and outer boundaries via 1) surfactants and 2) temperature. The shell confinement induces complex states and associated surface structures: a state where large stripes on the shell can be filled with smaller, perpendicular sub-stripes, and a focal conic domain (FCD) state, where thin stripes wrap into at least two, topologically required, double spirals. In this work, we focus on the latter state and use a Landau-de Gennes model of the CLC to simulate the detailed configurations of the FCD state as a function of anchoring strength. This work extends the knowledge of cholesteric patterns, structures that not only have potential for use as intricate, selfassembly blueprints but are pervasive in biological systems.

^{*}Speaker

Atomistic Simulation of Stacked Nucleosome Core Particles.

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Abstract

We report the first atomistic simulation of two stacked Nucleosome Core Particles (NCPs), with an aim to understand, in molecular detail, how they interact, the effect of salt concentration and how different histone tails contribute to their interaction, with a special emphasis on the H4 tail, known to have the largest stabilizing effect on NCP-NCP interaction. We do not observe specific K16-mediated interaction between the H4 tail and the H2A-H2B acidic patch, in contrast to the findings from crystallographic studies, but find that the stacking was stable even in the absence of this interaction. We perform simulations with the H4 tail (partially/completely) removed and find that the region between LYS-16 and LYS-20 of the H4 tail holds special importance in mediating inter-NCP interaction. Performing similar tail-clipped simulations with the H3 tail removed, we compare the roles of the H3 and H4 tails in maintaining the stacking. We discuss the relevance of our simulation results to the bilayer and other liquid crystalline phases exhibited by NCPs in vitro and, through an analysis of the histone-histone interface, identify the interactions that could possibly stabilize the inter-NCP interaction in these columnar mesophases. Through the mechanical disruption of the stacked nucleosome system using steered molecular dynamics (SMD), we quantify the strength of inter-NCP stacking in the presence and absence of salt. We disrupt the stacking at some specific sites of inter-nucleosomal tail-DNA contact and perform a comparative quantification of the binding strengths of various tails in stabilizing the stacking. We also examine how hydrophobic interactions may contribute to the overall stability of the stacking, and find a marked difference in the role of hydrophobic forces as compared to electrostatic forces in determining the stability of the stacked nucleosome system.

*Speaker

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Metastability in nematic liquid crystal shells

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Abstract

Confining a nematic to a spherical geometry inevitably yields topological defects. For example, nematic liquid crystals, constrained to lie parallel to the interface of a drop, possess two surface defects, called boojums. When a nematic is confined to a shell geometry, i. e. between two spherical surfaces, a number of different defect structures results from an interesting interplay between topological constraints and energy minimization [1,2]. Recent experimental results on nematic shells suggest that the existence of energy barriers, which separate one defect configuration from the others, can play a determinant role in stabilising metastable structures. [3,4] In this work, we show the existence of metastability in nematic shells. By imposing an external osmotic pressure, we change the shell average thickness to reach situations that are energetically unfavorable. We observe two different transition routes along the process. Remarkably, we observe a dramatic transition in which the inner droplet is expelled from the shell when a critical average thickness is reached. We find that the critical average thickness depends on the osmotic pressure of the outer phase.

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*Speaker

Molecular Dynamics of DNA aggregation

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Abstract

Various theoretical works have been performed in the past decade on interactions in strongly charged polyelectrolyte systems. It is interesting to explore the physics of self assembly of these systems, as it allows us to make strong connections to biological systems, which can give us insight to some of the fundamental questions of how a long DNA molecule (~ 1 m) can get compacted inside micron size nucleus (chromosomes). Also people have performed experiments on DNA condensation mediated by protamine and found that even at low concentration of condensing agent, increasing the salt concentration, they get precipitated phase of DNA. It is interesting because of the strong attraction exhibited between these strongly charged polyelectrolytes, mediated by counterions. We have studied the self assembly and condensation of different models of DNA, mediated by various condensing agents, using a coarse grained approach. We have also studied completely atomistic DNA-protamine system, to compare with results from coarse grained simulations, and to have a better understanding of the adsorption of protamine on an atomistic DNA.

*Speaker

Stem Cell-Encapsulating Colloidal Microgels with Tunable Biomechanical Cues for Tissue Regeneration under Inflammatory Microenvironments

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Abstract

Immunoisolation-based controlled delivery of exogenous stem cells has been a major technological challenge in tissue regeneration fields especially for the case of pro-inflammatory microenvironments in acute and chronic bone wounds. In this presentation, we report novel colloidal and injectable hydrogel microspheres, encapsulating mesenchymal stem cells (MSCs), which function simultaneously as a miniaturized delivery vehicle and bioengineered niche for MSCs. The microgel material was composed of a three-dimensional network of gelatin, mimicking mammalian extracellular matrices (ECMs), which was covalently crosslinked with genipin to minimize cytotoxicity. The genipin-crosslinked gelatin gel capsule efficiently shielded the embedded MSCs to maintain the cell viability over 95% in pro-inflammatory environments. Based on this cell protection, the gel matrix acted as an engineered ECM to regulate the MSC morphology and proliferation through tuning the elasticity of the gel matrix. Furthermore, degradation-mediated MSC release ability could be conferred to the microgel vehicles by tuning gel crosslinking degree. It was hypothesized that these unique properties are closely related to mechanobiological interactions between gel matrix and embedded MSCs.

*Speaker

Self-assembly of quantum dots in nematic and cholesteric liquid crystal shells

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Abstract

In recent years, the behaviour of micro- and nanometric particles embedded in liquid crystal media has received a lot of attention [1,2]. Indeed, anisotropic fluids such as liquid crystals can be used to direct the self-assembly of small inclusions, offering an easy and innovative way to manipulate them. Particles can be functionalized so that liquid crystal molecules align themselves perpendicularly to their surface. Under such perpendicular anchoring conditions, particles dispersed in a nematic phase are known to form chains oriented along the nematic director [3]. If defects are present in the field, the chains then migrate towards these areas of local disorder. Defects therefore act as privileged sites for liquid-crystal mediated self-assembly [4].

To stabilize defects, one strategy is to confine the liquid crystal to a spherical geometry under parallel boundary conditions. Indeed, the curvature of the confining space frustrates the orientational order and defects become topologically required. Previous studies report the inclusion of microparticles to drops and shells of liquid crystals, and their interactions with the topological defects [5,6].

In this ongoing work, we investigate experimentally the behaviour of quantum dots (QD) in drops and shells of liquid crystals. Using fluorescent and polarized light microscopy, we find that QD segregate at the liquid crystal / water interface and cluster in colloidal aggregates. At low QD concentrations, QD clusters localize at the defects, creating patches. At high QD concentrations, more intricate structures emerge. In nematic shells, QD clusters form chains, whose spatial arrangement and bending materializes the dipolar symmetry around the topological defects. In cholesteric drops – cholesteric liquid crystals are chiral nematics where the director spontaneously twists – they assemble in double spirals that wrap around the surface of the droplet, stemming from a radial defect line. Lastly, in cholesteric shells with perpendicular boundary conditions, they prevent closed defect lines from disappearing. In turn, they self-assemble along these lines, forming closed loops of QD clusters. We also study how the presence of the particles affects in turn the number and the position of the defects.

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Aqueous Amine CO₂ Capture Solutions: Molecular Dynamics Simulation

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Abstract

Chemical absorption of CO₂ by aqueous amine solutions is currently the most mature technology to capture CO₂ from post-combustion flue gases. A density-functional-theory-based fast virtual screening of the CO₂ capture performance has been developed for various aqueous amine solutions such as monoethanolamine (MEA) and piperazine (PZ). The important issues in developing high-performance amine solutions for CO₂ capture are a rapid increase of the viscosity of amine solutions containing PZ with the CO₂ loading as well as a evaporation lose of amine. A new design of a fast-CO₂-absorbing component as fast as PZ but not as viscous as PZ is therefore desirable. For this purpose, using molecular dynamics simulations combined with Green-Kubo (GK) and Stokes-Einstein (SE) methods, we compute the transport behavior (viscosity and diffusivity) of bulk aqueous amine solution as a function of CO₂ loading at different conditions as well as the interfacial properties (surface tension and vapor-liquid-equilibrium (VLE)) of gas-liquid interface with amine solution, and compare our findings to the experimental data. The result is compared to those of less problematic solutions such as MEA in order to unveil the microscopic origin of such a rapid viscosity increase of PZ. The calculation indicates that the SE method predicts higher viscosities than the GK method. The CO₂-loading-dependent viscosities calculated with the GK method and VLE curve and surface tension reproduce the experiments.

*Speaker

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Formation, Structure and aggregation of DNA toroids

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Abstract

We present two protocols to form DNA toroids : 1) DNA is simultaneously released from the bacteriophage capsids and condensed by spermine. These toroids are large and barrel shaped (about 300 nm in diameter) 2) A very dilute solution of plasmid DNA is condensed by addition of spermine. Small toroids are formed (50 -150 nm in diameter) that may secondarily aggregate by piling on top of each other. We describe the deviations from the perfect hexagonal ordering observed by cryo electron microscopy : double twist configurations are found in the smallest toroids, and more complex configurations in larger ones.

*Speaker

Chirality and frustration in large DNA toroids

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Abstract

Defects observed by cryoTEM in large DNA toroids are presented. We discussed the nature of these defects in line with theoretical predictions.

*Speaker