北京航空航天大學
BEIHANG UNIVERSITY

Outlook of Soft Matter Physics and Its Applications

软物质物理及其应用展望国际会议

15-18 December 2017 · Vision Hotel

Host：
Center of Soft Matter Physics and Its Applications
School of Chemistry
School of Physics and Nuclear Energy Engineering

Conference Program

15th Dec. 2017, 10:00-20:00 Registration, at the lobby of Vision Hotel		
16th Dec. 2017, the morning of Saturday • Vision Ball Room (4th floor)		
08:30-08:45	**Opening remarks.** **Host: Prof. Lei Jiang**	
08:45-09:15	**Photos time**	
First session: Chair **Prof. Zhongcan Ouyang**		
Time	**Speaker**	**Title**
09:15-09:45	**Ronald G. Larson** University of Michigan	The challenge of modeling thermodynamics and transport in gels and semi-crystalline materials
09:45-10:15	**Daan Frenkel** Cambridge University	Phoretic transport: a challenge for microscopic simulations
10:15-:10:45	**Ole Hassager** Denmark Technical University	Fracture in soft materials
10:45-11:05 Coffee break		
Second session **Chair: Prof. Yuliang Yang**		
11:05-11:35	**An-Chang Shi** McMaster University	Periodic and aperiodic order in soft matter systems
11:35-12:05	**Mark Matsen** University of Waterloo	Achieving quantitative predictions for block copolymer systems
12:05-12:35	**Kurt Kremer** Max Planck Institute for Polymer Research	Towards molecular control of physical processes in soft matter
12:35-14:00 Lunch break at Oasis Café(3rd floor)		

16th Dec. 2017, the afternoon of Saturday • Vision Ball Room (4th floor)		
Third session **Chair: Prof. Charles C. Han**		
Time	**Speaker**	**Title**
14:00-14:30	**Thomas P. Russell** University of Massachusetts Amherst	When liquids are liquids
14:30-15:00	**David Andelman** Tel Aviv University	One hundred years of the poisson-boltzmann theory: some recent developments and outlook on charged soft matter
15:00-15:30	**Raphael Blumenfeld** Imperial College London	Granular statistical mechanics: bridging between statics and dynamics
15:30-15:50 Coffee break		
Forth session **Chair: Prof. Pingwen Zhang**		
15:50 -16:20	**Steve Granick** University of Illinois	Surprises while watching single macromolecules in real time
16:20-16:50	**Penger Tong** Hong Kong University of Science and Technology	Colloidal diffusion over complex potential landscapes: from periodic, quasi-periodic and random potentials to live cell membranes
16:50-17:20	**Charles C. Han** Shenzhen University	From dynamics of the glass tranformation of structural materials to the interactive phase separation and crystallization in a dynamically asymmetric polymer blend
18:00 Banquet at Dongfanghong Restaurant		

17th Dec. 2017, the morning of Sunday • Vision Ball Room (4th floor)

First session
Chair: Prof. Masao Doi

Time	Speaker	Title
09:00-09:20	**Xiangyang Liu** Xiamen University National University of Singapore	Two-step intra/inter molecular nucleation of silk fibroin materials and mesoscopic engineering
09:20-09:40	**Er-Qiang Chen** Peking University	Interplay of main- and side-chain in side-chain fiquid crystalline polymers
09:40-10:00	**Tiezheng Qian** Hong Kong University of Science and Technology	Reciprocal theorem: from local equations to symmetry over the whole system
10:00-10:20	**Dadong Yan** Beijing Normal University	Local-jump model of polymer crystallization

10:20-10:40 Coffee break

Second session
Chair: Prof. An-Chang Shi

Time	Speaker	Title
10:40-11:00	**Wenbing Hu** Nanjing University	Effect of sequence defects on the free energy change of intramolecular polymer crystallization
11:00-11:20	**Zhao-Yan Sun** Changchun Institute of Applied Chemistry, Chinese Academy of Sciences	Structure and dynamics of glass-forming liquids
11:20-11:40	**Ping Tang** Fudan University	Phase transition behavior in self-assembled rod-coil block copolymers
11:40-12:00	**Chenxu Wu** Xiamen University	Topological dependence of polymer brushes

12:00-14:00 Lunch break at Oasis Café (3rd floor)

17th Dec. 2017, the afternoon of Sunday • Vision Ball Room (4th floor)

Third session
Chair: Prof.Xuefeng Yuan

Time	Speaker	Title
14:00-14:20	**Baohui Li** Nankai University	Precise control of self-assembly of complex polymer systems
14:20-14:40	**Weihua Li** Fudan University	To design block copolymers for desired ordered structures or even properties?
14:40-15:00	**Li-Tang Yan** Tsinghua University	Understanding diffusion dynamics of nanoparticles on cell membrane through theory and simulation
15:00-15:20	**Hujun Qian** Jilin University	Dynamics in polymer/single-chain nanoparticle composites

15:20-15:40 Coffee break

Forth session
Chair: Prof. Jeff Chen

15:40-16:00	**Fangfu Ye** Institute of Physics, Chinese Academy of Sciences	Emergent edge flow of active rotor mixtures
16:00-16:20	**Zhong-Yuan Lu** Jilin University	Challenges in coarse-grained simulations of polymer systems at larger spatiotemporal scales
16:20-16:40	**Hongxia Guo** Institute of Chemistry, Chinese Academy of Sciences	Nanoparticles in directing the compatibilization behavior and the morphological transition of immiscible polymer blends under shear flow
16:40-17:00	**Kai Yang** Soochow University	Complicated activities related to cell membranes
17:00-17:20	**Zhengdong Cheng** Texas A&M University Guangdong University of Technology	Dynamics of colloidal mixtures and control
17:20-17:40	**Feng Liu** Shanghai Jiao Tong University	Printing and in-situ morphology observation of organic photovoltaics

18:00 Farewell dinner at Oasis Cafe(3rd floor)

18th Dec. 2017, Departure

Ronald G. Larson

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The Challenge of Modeling Thermodynamics and Transport in Gels and Semi-Crystalline Materials

Abstract: Many relatively common materials, including semi-crystalline polymers, drug-polymer composites used in oral drug delivery, shampoos and other consumer products, and latex paints, contain multiple components or multiple phases that defy conventional treatments of equilibrium or transport. Such materials are therefore frequently designed by trial-and-error or ad hoc principles by industry. New tools promise to change this picture, by using a combination of advanced theory, high-speed and multi-scale computing, and new methods of sampling equilibrium and transition paths. Examples will be discussed where results are very limited, but progress is now possible, including predicting crystallization of drugs in the presence of polymer excipients, predicting the rheology of polymer-containing latex dispersion networks or networks of surfactant micelles, and crsytallization under flow of semi-crystalline polymers such as polyethyelene. An outline of a process of linking simulations and theories over multiple scales will be proposed for dealing with such materials.

Daan Frenkel

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Phoretic Transport: a Challenge for Microscopic Simulations

Abstract: Nanotechnology is not just conventional technology scaled down to the nano-scale. The reason is that processes that are relatively unimportant on macroscopic scales may become dominant on the nano-scale. Case in point are phoretic flows: the movement of fluids under the influence of gradients of thermodynamic quantities such as > temperature or chemical potential. On a macroscopic scale, the application of a pressure gradient or a body force is the most efficient way to move fluid through a tube. The resulting flux is proportional to the fourth power of the tube diameter. However, on a sub-micron scale, phoretic flows tend to become important because the resulting volumetric flow rates scale as the square of the tube diameter. Hence, for many problems, be they chnological (e.g. nano-fluidics) or natural (e.g. fluid flow through porous networks or gels), it is becoming increasingly important to be able to model phoretic flows.

It turns out that, whilst the local continuum description of phoresis is straightforward, there are real problems with a fully microscopic approach that is needed in predictive molecular simulations.

In my talk, I will discuss different approach to computing phoretic flows and show what works, and more interestingly, what fails.

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Fracture in Soft Materials

Abstract: Fracture is a phenomenon that is generally associated with solids. A key element in fracture theory is the so-called weakest link idea that fracture initiates from the largest pre-existing material imperfection. However, recent work has demonstrated that fracture can also happen in liquids, where surface tension will act to suppress such imperfections. Therefore, the weakest link idea does not seem immediately applicable to fracture in liquids. This presentation will review fracture in liquids and argue that fracture in soft liquids is a material property independent of pre-existing imperfections. The following questions then emerge: What is the material description needed to predict crack initiation, crack speed and crack shape in soft materials and liquids.

An-Chang Shi

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Periodic and Aperiodic Order in Soft Matter Systems

Abstract: The observation of ordered phases in condensed matter systems such as metallic alloys has a long history in materials physics. In recent years, intricate periodic and aperiodic order has emerged in a host of soft matter systems including supramolecular assemblies, surfactants and block copolymers. The occurrence of complex phases in these diverse systems underscores the universality of emergent order in condensed matter. For the case of block copolymers, recent experimental and theoretical studies have revealed that non-classical ordered phases, such as quasicrystals and the Frank-Kasper and Laves phases, could emerge from block copolymers as equilibrium or metastable morphologies. As such, block copolymers provide an ideal system to study the origins and stability of periodic and aperiodic order in condensed matter physics. In my presentation, I will summarize recent theoretical and experimental progresses on this fascinating topic and discuss possible future research directions.

Mark Matsen

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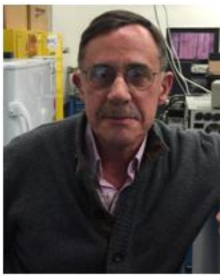
Achieving Quantitative Predictions for Block Copolymer Systems

Abstract: Ideally, we would like to have first-principles simulations capable of quantitatively accurate predictions for any block copolymer system. Usually, our choice of model involves balancing the complexity needed to faithfully represent an actual experimental system and the simplicity required to make the simulation tractable. Fortunately, block copolymer phase behavior is believed to become universal in the high molecular-weight limit, which foregoes the need for detailed models. We illustrate how this universality can be used to make accurate predictions for a diblock copolymer melt from simulations using a simple lattice model. Nevertheless, simulations of blends and/or complex architectures are still extremely challenging even with the simplest of models. We conclude by discussing how this last obstacle could be overcome with field-theoretic simulations.



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When Liquids are Liquids

Abstract: Liquids have the many desirable characteristics, including rapid transduction of energy carriers (both charged and neutral), conformability to arbitrary shapes, and controlled dissipation of mechanical energy. Yet, being fluid, liquids do not hold shape and, as such, it is not possible to spatially direct these desirable features without solid confinement. Using a very simple concept, i.e. the formation, assembly and jamming of nanoparticles surfactants at fluid interfaces, we have been able to effectively structure liquids wherein all the desirable characteristics of the liquids can be retained but the liquids can be shaped with the structural stability of a solid. The spatial and temporal characteristics of structured liquids span from the nanoscopic to macroscopic, over many orders of magnitude in time, making these systems mesoscopic in space and time. We have developed strategies to control individual nanoparticle chemistries and their assembly and dynamics at interfaces to cascade events on the nanoscopic level to the macroscopic level. The nanoparticle surfactant assemblies respond to external stimuli giving rise to a new family of adaptive materials. Systems raging from bijels to molded liquids to 3D printed systems have been developed were the systems are fully liquid but have a robust structure that can evolve in time in response to internal and external forces.

David Andelman

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One Hundred Years of the Poisson-Boltzmann Theory: Some Recent Developments and Outlook on Charged Soft Matter

Abstract: Roughly a century has passed since the seminal works of Gouy, Chapman, Debye and Huckel addressing the behavior of mobile ions in solutions and close to charged interfaces. In this talk, I will briefly review the state-of-the-art of the resulting Poisson-Boltzmann theory that is even today the benchmark of modeling charges in aqueous media, with numerous application in soft and biological matter. Then, I will address more recent modifications and extensions of the Poisson-Boltzmann theory, including steric effects and non-electrostatic specific ionic effect, the molecular dipolar nature of the solvent (usually water), as well as taking into account correlations and fluctuations beyond the Mean-Field treatment. Finally, I will propose several unexplored directions which may lead to new and exciting development to the one-hundred-year-old theory.

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Granular Statistical Mechanics: Bridging Between Statics and Dynamics

Abstract: A first-principles statistical mechanics is formulated for slow dense granular fluids, where prolonged intergranular contacts vitiate collision theory. The contacts are regarded as virtual particles, exchanged during the dynamics between different structure types.

These types, characterized by different mean coordination numbers, have different contact potentials, which are analogous to chemical potentials of reacting chemical species.

Significantly, this formalism converges to the connectivity-based static statistical mechanics when the motion stops, thus bridging between static and dynamic granular mechanics.

The theory is illustrated on a sheared granular system. Expectation values are derived for the mean and variance of the coordination number distribution, as well as a relation between the contact potentials and the shear rate.

Steve Granick

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Surprises While Watching Single Macromolecules in Real Time

Abstract: A fundamental challenge of modern physical science is to form structure that is not frozen in place but instead reconfigures internally driven by energy throughput and adapts to its environment robustly. Predicated on fluorescence imaging at the single-particle level, this talk describes quantitative studies of how this can happen. With Janus colloidal clusters, we show the powerful role of synchronized motion in self-assembly. In living cells, we find that transportation efficiency problems bear a provocative parallel with polymer chain trajectories with their spatial extent, and with jammed matter in their time evolution. A picture emerges in which simple experiments, performed at single-particle and single-molecule resolution, can dissect macroscopic phenomena in ways that surprise.

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Colloidal Diffusion Over Complex Potential Landscapes: From Periodic, Quasi-Periodic and Random Potentials to Live Cell Membranes

Abstract: Energy landscape is an important concept in science, which has been widely used in many areas of physics, chemistry, biology and materials science. Applications of the energy landscape concept can be found in the calculation and measurement of the chemical reaction rate, lifetime of single molecular bonds, folding kinetics of proteins, and phase diagram of complex materials. Our general understanding of this type of problem is through the well-known Arrhenius-Kramers equation, which was obtained under an idealized condition for a single energy barrier. For many practical applications, however, one often encounters complex energy landscapes. There are few experimental systems in which one can actually visualize the energy landscape, and thus much of the work done so far is through computer simulations. A physical model system in which one can directly measure the energy landscape and track individual particle trajectories would be extremely valuable in testing different theoretical ideas. In this talk we will present our recent efforts in developing a two-layer colloidal system to study colloidal transport and dynamics over complex potential landscapes [1-3]. This work opens up a whole new realm of investigation at the single-particle level for a range of interesting problems associated with the diffusive and forced barrier-crossing dynamics over complex energy landscapes. Examples of applications of this system will be discussed.

[1] "Colloidal diffusion over a periodic energy landscape," X.-G. Ma, P.-Y. Lai, and P. Tong, Soft

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From Dynamics of the Glass Tranformation of Structural Materials to the Interactive Phase Separation and Crystallization in a Dynamically Asymmetric Polymer blend

(Future challenges, directions, and opportunities in soft matter)

Abstract: In this talk, the glass transition of structural materials, especially for polymers, colloids and colloid/polymer systems will be presented. The splitting and non-proportional slowing down in relaxation processes of structural materials will be emphasized. A simple example of particles with a repulsive potential plus a short range attraction will be used to illustrate the bridging and jamming structures that could be the key structural characteristics which leads to various dynamic features during the glass transformation, such as: modes slowing down, (dynamic) free volume change, local heterogeneity, and etc.

By observing the experimental results from such an explicit model system which emulates a measurable and visible molecular model of structural glass, we will give our interpretation on a molecular picture and the dynamic slowing down on the glass transition of colloids and polymers. We will also make some reviews and observations about the most popular theories: 1) Free volume theory, 2) Entropy theory, 3) Götze Mode coupling theory, and 4) Caging and Jamming theory.

Then, we will give two examples for current and future directions in applications:

Example I:

Utilization simultaneous or interactive transitions of crystallization and phase separation in an asymmetrical binary blend which uses the slower relaxation mode to control the structural or morphological evolution could add a new dimension in polymer processing. An example of a

dynamically asymmetric poly(methyl methacrylate) (PMMA) and poly(ethylene oxide) (PEO) blend will be used to illustrate this process.

Example II:

Glass transition controlled Electro-spun fibrous membrane as a Category III bio-medical devices for delivery of multi-functional applications.

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Two-Step Intra/inter Molecular Nucleation of Silk Fibroin Materials and Mesoscopic Engineering

Abstract: This talk is to show how the concepts and ideas of crystallization can be further extended and applied to the field of mesoscopic soft materials, ie. silk fibroin materials. It concerns the structural characteristics vs the macroscopic performance, and the formation mechanism of intra molecular crystal networks. Firstly, the occurrence of hierarchical structure, c.f. crystal network and domain network structures, will facilitate the formation kinetics of mesoscopic phase, and boost up the macroscopic performance of materials in some cases (i.e. spider silk fibres). Secondly, the structure and performance of materials can be correlated in some way by the four factors: topology, correlation length, symmetry/ordering, and strength of association of crystal networks. Moreover, four different kinetic paths of crystal network formation are identified, namely, one-step process of assembly, two-step process of assembly, mixed mode of assembly and foreign molecule mediated assembly. The detailed mechanism of two-step intra/inter molecular nucleation will be addressed based on combined. technologies, atomic microscopy, circular dichroism, FTIR, SAXS, etc. This allows the rational design and construction of the mesoscopic structure in flexible mesoscopic materials. In this context, the (re-)construction of hierarchical crystal network structure can be implemented by thermal, participate, chemical, sonication stimuli etc. Based on this principle, the new technologies, i.e., meso-functionalization, meso-fabrication can be developed, which can lead to a new class of flexible meso comments. This will play a significant role in biomedical applications in the years to come.

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Interplay of Main- and Side-Chain in Side-Chain Liquid Crystalline Polymers

Abstract: As a typical soft matter and important functional materials, side-chain liquid crystalline polymers (SCLCPs) exhibit pronounced heterogeneities of chemistry and dynamics of their main- and side-chain. Therefore, the essential of SCLCP research is to understand and manipulate the interplay of main- and side-chain. Introducing a flexible spacer between the main-chain and mesogenic pendant group can decouple the motions of main- and side-chain. The "decoupling" effect facilitates the formation of liquid crystal (LC) phases that are largely dependent on the property of mesogenic groups. On the other hand, laterally attaching the rod-like or other bulky side-chain to the main-chain through a very short linkage or even a single carbon-carbon bond can result in a strong "jacketing" effect, making the main- and side-chain integrated together. Consequently, the whole chain, which is quite extended and either rod- or lath-like, becomes the building block for the LC structure. Combining "decoupling" and "jacketing" effect can pave a way towards new LC materials with fascinating hierarchical structures. To further tune these two effects, we consider that the length of flexible backbone between two adjacent side-chains, i.e., the side-chain spacing, can be the key factor. Its influence on the structure and dynamics of SCLCP has not been systematically investigated so far. We anticipate that the variation of side-chain spacing and thus the side-chain density will give SCLCP more interesting and complex self-assembly behaviors invoking the competition of microphase separation, LC transition, crystallization, etc., based on which SCLCP functional materials with unique viscoelastic properties can be fabricated.

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Reciprocal Theorem: From Local Equations to Symmetry Over the Whole System

Abstract: Onsager's reciprocal symmetry is typically used to derive local constitutive equations through a variational approach. We consider a non-equilibrium system close to the global equilibrium state. We show that the reciprocal symmetry for local constitutive equations can be extended to a new symmetry over the whole system. This symmetry is manifested in the kinetic coefficients connecting the forces and fluxes defined at the system boundary. Our results generalize the Lorentz theorem for Stokes flows.

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Local-Jump Model of Polymer Crystallization

Abstract: The structure of crystal-amorphous interface of folding surface controls the properties of the polymer lamellar crystal. The interfacial tension is heavily dependent on the persistence length and the distance between two injection points. The polymer segments release the interfacial tension by perpendicular local jump of chain stems. As a consequence, for a given thickness of interfacial layer, the optimal interfacial structure depends on the distribution of the injection points. In the present work, a local-jump model based on the worm-like chain model is developed to investigate the effects of lateral motion of stems in the crystal region during polymer crystallization for the first time, which provides a theoretical explanation for the intrinsic length scales (the thickness of interfacial layer, and the distance between two injection points) of the interfacial structure, which were ignored in all the previous theories. The crystal-amorphous interfaces comprised both of tight folds and of loose loops are studied by single-chain in mean-field theory (SCMFT). Wang-Landau algorithm is applied to obtain accurate solution of partition function in both SCMFT and Muthukumar's theory which is given theoretically by single Gaussian chain model. For various loop length, the optimal distance between two injection points is determined by the balance of chain stiffness and conformational entropy. All the results provide evidences to the tight-folded model. A possible explanation involving density of injection points is proposed to interpret the mechanism of bias for this model. Besides, to satisfy the requirement of calculation for both the information completeness in global energy space and the information precision in local low-energy states synchronously, a three-step high-precision Wang-Landau algorithm is developed and turns out to be high-feasible.

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Effect of Sequence Defects on the Free Energy Change of Intramolecular Polymer Crystallization

Abstract: The sequence defects on polymer chains significantly suppress the crystallinity for a broad application, for examples, the short branches on polyethylene from plastics to elastomers, and the stereo-isomers on polypropylene from fibers and plastics to adhesives. We performed dynamic Monte Carlo simulations of single linear and cyclic polymer chains containing a few of sequence defects. The changes in the free energy curves of intramolecular crystallization/melting show that the sequence defects generally suppress the melting points from the corresponding linear and cyclic homopolymer chains, but affect little to the kinetic barrier for intramolecular crystal nucleation. In addition, the chain ends play the similar role as the sequence defects in crystallization. The results shed light onto our better understanding of sequence-length segregation upon crystallization of statistical copolymers. We thanks the financial support of NNSFC (Grant No. 21474050 and 21734005).

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Structure and Dynamics of Glass-Forming Liquids

Abstract: The nature of glass transition is one of the most poorly understood mysteries in physics. Upon cooling, glass forming liquids display markedly slow and heterogeneous dynamics but unperceivable change in its static structures. Although intense attention has been paid to explore the structural origin of slow dynamics and dynamical heterogeneity, a more convincing view is still lacking and the relationship between structure and dynamics seems to be quite complex. In this presentation, I will review some recent viewpoints on the relation between structure and dynamics, and I will also propose a locally preferred structural order to describe the structure characteristics of glass-forming liquids, which may provide some hints to help understand the relationship between structure and dynamics.

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Phase Transition Behavior in Self-assembled Rod-coil Block Copolymers

Abstract: By combining the string method with the self-consistent field theory for the polymeric system with chain rigidity, we aim to study order-order phase transition kinetics, including the minimum energy pathways, the emergence of various metastable states and their dependence on these pathways. By designing different initialization procedures of the "string", we wish to investigate the epitaxial relationship between distinct phases, the nucleation details including the shape, size of the critical nucleus and nucleation barrier, and the stability of the metastable states. Furthermore, we expect to regulate the kinetic pathways to complex spherical packing phases, and multiply continuous networks with liquid crystal orientation effect. The developed theoretical method is expected to understand the phase transition mechanism regarding complex self-assembled networks and liquid crystalline phases, thus providing guidance for the design and fabrication of high performance and functional materials.

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Topological Dependence of Polymer Brushes

Chanfei Su, Wubin Wan, Holger Merlitz, and Chenxu Wu

Abstract: Molecular dynamics simulations were performed to study the topological dependence of polymer brush. Both ring and starlike polymer brushes are investigated, and a comparison with those of linear polymer brush is also made. It is found that there exists a master scaling power law of the total stretching energy scaled by chain length, for moderate chain length regime, for ring polymer brushes, but with a larger exponent than 5/6, indicating an influence of topological constraint to the dynamic properties of the system. We also investigate the structural properties of binary polymer brushes, composed of functional 4-armed star polymers and chemically identical linear polymers of different molecular weights. The molecular dynamics simulations confirm recent self-consistent field studies, in which a considerable potential of these systems for the design of switchable surfaces has been claimed. The length of the linear chains serves as a control parameter, which, while passing over a critical value, induces a sharp transition of the molecular conformation. These transitions at different grafting densities are studied and summarized in a phase diagram.

Keywords: polymer brush, topological dependence, star-like, ring, binary

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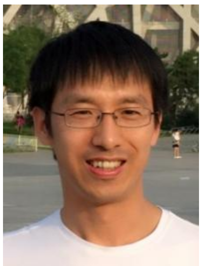
Precise Control of Self-assembly of Complex Polymer Systems

Abstract: Self-Assembly processes are ubiquitous in nature. These processes occur without external intervention and can create complex heirarchical structures through the statistical exploration of alternative configurations of building blocks. Self-assembly of molecules or macromolecules constitutes a “bottom-up” approach to generate technologically important materials. This ability to manufacture nanomaterials with complex and structured composition through self-assembly of polymers increasingly underpins the next generation of technologies.

Block copolymers are a class of soft material capable of self-assembling to form ordered structures at nanometer scales, providing potential for a wide variety of applications. The self-assembled structures from block copolymer systems are exquisitely sensitive to temperature, composition, solvent, external field, enclosing boundaries or other associated variables. Therefore, one may control the domain orientation or morphology of the self-assembled structures by adjusting these variables. In this line, many progresses have been achieved. Block copolymer systems, on the other hand, provide a paradigm studying self-assembly.

Precise control of self-assembly of complex polymer systems, however, remains a bottleneck due to the large number of parameters involved in the system. In my talk, I will list a few such complex polymer systems, and discuss their self-assembling behaviour.



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To Design Block Copolymers for Desired Ordered Structures or Even Properties?

Abstract: In a condensed matter system, the structure usually dictates its physical properties. In turn, the condensed structure is dictated by the structure of molecules. Specifically, for block copolymer, the self-assembled structure is solely determined by the chain architecture, i.e. topology and composition, when the composed species are given. It would be particularly useful if we could design the architecture of block copolymers for desired ordered structures or even physical properties. The key step for the design of block copolymers is to build up some valid guiding principles. In recent years, we have proposed a few useful guiding principles: adjustable bridging blocks, combinatorial entropy, conformational asymmetry, and local segregation. Abiding by these principles, a number of block copolymer systems are successfully designed, leading to many non-classical ordered structures, including rich binary mesocrystals, a square array of single-component cylinders, complex Frank-Kasper spherical packing phases, dodecagonal quasicrystal approximant, hybrid lamella-sphere phase, etc. If some novel structures for targeted physical properties are desired, this concept of inversely designing block copolymers may be further extended, thus going through the complete inverse-design procedure from physical properties to condensed structures and then to molecular structures.

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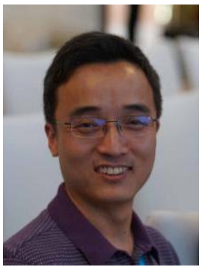
Understanding Diffusion Dynamics of Nanoparticles on Cell Membrane Through Theory and Simulation

Abstract: The transport of nanoparticles at the bio-nano interfaces is essential for many cellular responses and biomedical applications. How two-dimensional nanomaterials, such as graphene and transition-metal dichalcogenides, diffuse along the cell membrane is, however, unknown, posing an urgent-important issue to promoting their applications in biomedicine. Here we show experimentally and theoretically that the diffusive transport of graphene nanosheets (GNs) sandwiched inside cell membrane varies from Brownian dynamics to Lévy walks and even directional motion. Specifically, experiments evidence the sandwiched graphene-cell membrane superstructures predicted by simulations. Combined simulations and experiments identify sandwiched-GN-induced pore in the leaflets of cell membrane, spanning unstable, metastable, and stable states. Analytical model that rationalizes the regimes of these membrane-pore states fits the simulations quantitatively, leading to a mechanistic interpretation of the emergence of Lévy and directional dynamics. Our findings inform approaches to program intramembrane transport of two-dimensional nanomaterials, and suggest design principles for novel composite systems integrating such emerging nanomaterials inside biological membranes.



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Dynamics in Polymer/Single-Chain Nanoparticle Composites

Abstract: Properties of a polymer melt can be largely augmented by incorporating nanometer-sized particles. For instance, adding a small amount of nanoparticles (NPs) into polymer melt can often lead to a large change (either reduction or enhancement) in melt viscosity. A reduction in viscosity can not only improve the processability of the material but also favors the energy conservation during the relevant industrial processes. However, the underlying mechanism for such viscosity reduction (VR) remains a major mystery in the polymer field.

In this report, I will firstly report a recent finding in our group for a polymer composite system formed by linear polystyrene (PS) chains and single-chain PS NPs. By performing large-scale molecular dynamics simulations and experimental rheology measurements, we find that with a fixed loading of the NP, VR effect can be largely boosted up with an increase in matrix chain length N. A small amount of NP addition in long chain melt can cause a dramatic reduction in viscosity. Though NP induced disentanglement effect is observed in the system, it is only linearly proportional to the NP loading and can not fully account for the observed large VR effect. Instead, we will show that such VR is highly related to the high diffusivity of the NPs and an acceleration effect in the melt polymer chain dynamics at the NP surface area. In addition, we will also show that the chain dynamics in this system have a strong discrepancy from the prediction of the widely accepted tube model, i.e., chain relaxation time (τ) or viscosity (η) are observed to have a power law of $\tau \sim N^{\nu}$ (or $\eta \sim N^{\nu}$) with $\nu < 3$, which is in a strong contrast to $\tau \sim N^3$ predicted from tube theory or $\eta \sim N^{3.4}$ often observed experimentally for pure polymer melts. With the above results, a brief outlook of the challenges and opportunities will be given at the end of my talk.

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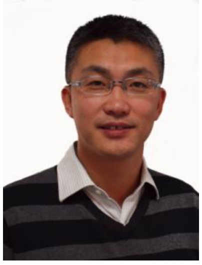
Emergent Edge Flow of Active Rotor Mixtures

Ying Zeng, Mingcheng Yang, Fangfu Ye

Abstract: Emergent collective phenomena is one of the most fascinating and intricate features in active matter. Here, we explore the collective behaviors of an active rotor mixture in confinement. The mixture consists of two components of rods with different spinning velocities. We find the emergence of an edge flow parallel to the boundary for each component. Strikingly, the emergent flows exhibit a significant oscillation and even change direction upon varying the distance to the boundary. Furthermore, the two emergent flows behave independently rather than compete against each other, although their constituent rotors interact strongly. Based on the interplay between the rod-rod interactions, spin, confinement and system compressibility, we then propose a microscopic mechanism to explain the simulation results.



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Challenges in Coarse-Grained Simulations of Polymer Systems at Larger Spatiotemporal Scales

Abstract: Due to large molecular size and the corresponding slow relaxation of polymer chains, a great amount of issues related to long-distance chain displacement (such as phase separation and self-assembly) cannot be tackled easily with conventional molecular dynamic simulations. There is urgent need to develop coarse-grained models at different length scales to scrutinize structural and dynamic characteristics of a complex polymer system. In my opinion, the challenges (some of them are actually not new) in the forthcoming decade may include: (1) develop robust coarse-graining method/algorithm at different length scales for polymer simulations, (2) develop coarse-grained simulation programs that can be allocated on next-generation many-core computers for large and massive simulations, (3) incorporate chain entanglement in coarse-grained simulations in an efficient way, and (4) use "self-learning" robots (machine learning) to build up coarse-grained polymer models.

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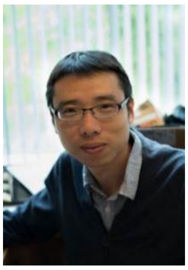
Nanoparticles in Directing the Compatibilization Behavior and The Morphological Transition of Immiscible Polymer Blends Under Shear Flow

Abstract: Blending polymers is a practical and simple means as to design new materials with beneficial properties of the individual components. There is a constant search for efficient compatibilizing agents, which allow for a sufficient mixing of the incompatible components with a compatibilizer content as low as possible. With the recent development in particle synthesis a large variety of nanoparticles, characterized by different surface properties and shapes, can be generated. Now, besides copolymers, adding nanoparticles (denoted by NPs) is taken to be an alternative approach to stabilize the immiscible polymer blends, wherein not only the interfacial adhesion and mechanical properties of polymer blends would be improved but also advantageous electrical, magnetic or optical properties of nanoparticles would be incorporated. Particularly, the surface properties of nanoparticles manipulate their positional distribution inside the polymer blends, and hence offer a high control for engineering polymer nanocomposite with desired structures and properties. Recent studies have shed more light onto the close relation between surface chemistry of NPs and their compatibilizing capability in polymer blends, however the understanding of how NPs control the miscibility behavior and the morphology of polymer blends is far from complete. Additionally, in many polymer-processing operations, shear flow is usually involved. Normally, in immiscible binary mixtures the shear flow affects the phase transitions and induce mixing or demixing by shifting the phase boundaries, which improves or weakens the component compatibility and also changes the morphology as well as stability of the domain. Actually, these effects arise from the coupling between kinetics, thermodynamics, hydrodynamics, and even viscoelasticity, and depend strongly on the applied processing condition as well as blend

composition and so on. In comparisons to researches in the area of the ternary blends (two immisicible homopolymers and one copolymer), to our best knowledge, investigations on the effect of shear flow on the behavior of phase-separating homopolymers containing nonoparticles are rather scarce, although nanoparticles offer an effective and economic alternative to the conventional method of compatibilizing polymer blends by copolymers. Considering the differences between copolymers and nanoparticles, introducing nanoparticles into an immiscible polymer blend could make the whole sample to undergo qualitatively different morphological transformations under flow. The resulting phase behavior may become more complex as these particles can be selectively located in the homopolymer phases or at the interface depending on their surface chemistry. Therefore, the ternary blends containing nanoparticles with different surface chemistry or shapes are highly interesting systems to study. A knowledge of the variational response of these systems to shear flows opens up possibilities for the rational design and fabrication of ordered nanostructures and advanced nanocomposites.



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Complicated Activities Related to Cell Membranes

Abstract: In this report, I will talk about some challenges facing the investigations on cell membrane activities, specifically from the perspective of molecular simulations. Membrane activity is one of the fundamental factors in realizing cellular functions, and is crucial in many processes in biomedical engineering. Unfortunately, the molecular mechanisms of most membrane behaviors are far from fully understood yet. Here, several examples will be involved, including the cellular endocytosis, transmembrane signaling and energy transfer. Additionally, effective combination of experiments and simulations, which has been challenging but promises attractive advantages in related studies, will be discussed.

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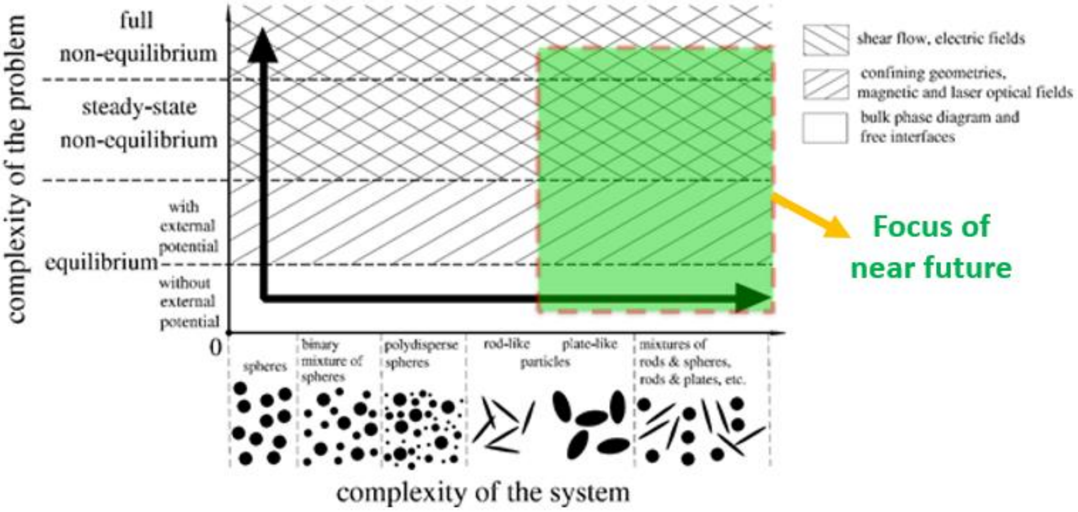
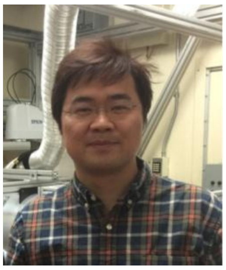
Dynamics of Colloidal Mixtures and Control

Abstract: The near future research of colloids and soft matter will expand in two dimensions: complexity of the system incorporating different shapes and degree of mixing, and complexity of the problem towards non-equilibrium. Dispersions of colloidal particles (size from 1 nm to a few microns) in a solvent are the simplest prototype of soft matter. Exciting questions concern collective many-body effects induced by cooperation and self-organization of many particles, including phase transitions, gelation and glass formation. The unique length scale (facilitates direct observation using optics) and time scale (milliseconds to days, very convenient for observation), and the easy to tailor the inter-particle interactions, enable colloids for fundamental research and technological development. Our group carries out the research of the liquid crystals of the nanoplates due to our capability to produce plates with extremely high aspect ratio, identical thickness (i.e. monolayers obtained by exfoliation of inorganic crystals), uniform in lateral size, and flexible to tailor the surface chemistry hence inter-plate interactions. Motivated by microscopic understanding, on the basic time and length scales, of molecules and colloids in non-equilibrium, colloidal mixture dynamics and control have become the frontier of current research activities.



Focus of near future

Complexity of colloidal systems (after Eur. Phys. J. Special Topics 222, 2013, 2727)



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Printing and In-Situ Morphology Observation of Organic Photovoltaics

Abstract: The solvent-processibility of polymer semiconductors is a key advantage for the fabrication of large area, organic bulk-heterojunction (BHJ) photovoltaic devices. Most reported power conversion efficiencies (PCE) are based on small active areas (~ 0.1 cm^2), fabricated by spin-coating technique. In general, this does not reflect device fabrication in an industrial setting. To realize commercial viability, devices need to be fabricated in a roll-to-roll fashion. The evolution of the morphology associated with different processing parameters, like solvent choice, concentration and temperature, needs to be understood and controlled. We developed a mini slot-die coater, to fabricate BHJ devices using various low band gap polymers mixed with phenyl-C71-butyric acid methyl ester (PCBM). Solvent choice, processing additives, coating rate and coating temperatures were used to control the final morphology. Efficiencies comparable to lab-setting spin-coated devices are obtained. The evolution of the morphology was monitored by in situ scattering measurements, detecting the onset of the polymer chain packing in solution that led to the formation of a fibrillar network in the film.

交通示意图：


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致真大厦
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