# 2017 International Workshop of A3 Foresight Program on Soft Matter

supported by A3 Foresight Program and Research Institute of Mathematical Science of CNU.

Dates: December 19-21, 2017

Venue: Room 1204, Building W-5, College of Natural Science,

Chungnam National University, Daejeon 34134, South Korea

Scientific Committee: Hyeonbae Kang , Inha University, Korea

Yasumasa Nishiura, Tohoku University, Japan

Pingwen Zhang, Peking University, China

Organizers: Jinhae Park, (Research Institute of Mathematical Science, CNU)

Jaeup Kim, UNIST,

Masao Doi, Beihang University, China

Natsuhiko Yoshinaga, Tohoku University, Japan

# Time Table

## Day 1 December 19, 2017

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|---|---|
| 09:00 ~ 10:00 | Meeting for Future A3 Foresight Program on Soft Matter |
| 11:00 ~ 13:00 | Registration and Lunch |
| 13:00 ~ 13:10 | Welcoming Remarks |
| 13:10 ~ 14:10 | Special Lecture (chair: Jinhae Park) |
| 14:10 ~ 17:00 | Afternoon session (chair, Natsuhiko Yoshinaga) |

## Day 2: December 20, 2017

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|---|---|
| 09:00 ~ 10:00 | Special Lecture (chair: Xingkun Man) |
| 10:00 ~ 12:10 | Morning Session (chair: Masao Doi) |
| 12:10 ~ 13:30 | Lunch |
| 13:30 ~ 14:30 | CNU Interdisciplinary Distinguished Lecture Series |
| 15:00 ~ 17:40 | Afternoon Session (chair: Jonghyun Kim) |
| 18:00 ~ 20:30 | Banquet |

## Day 3 December 21 2017

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|---|---|
| 09:00 ~ 10:00 | Special Lecture (chair: Hirofumi Notsu) |
| 10:00 ~ 12:10 | Morning Session (chair: Jaeup Kim) |
| 12:10 ~ 14:00 | Lunch |
| 14:00 ~ 17:30 | Afternoon Session |
| 17:30 ~ 17:40 | Closing Remarks |

| **Day 1: December 19, 2017** | | |
|---|---|---|
| **Time** | **Title** | **Speaker** |
| 11:00 ~13:00 | Registration and lunch | |
| 13:00 ~ 13:10 | Welcoming remarks | Jinhae Park, Chungnam National University |
| 13:10 ~ 14:10 | Special lecture: Onsager's principle 1 | Masao Doi, Beihang University |
| 14:10 ~ 15:00 | The drying of liquid droplets | Xingkun Man, Beihang University |
| 15:00 ~ 15:20 | Coffee Break | |
| 15:20 ~ 17:00 | Novel dynamics in systems of microtubules and kinesin motor proteins | Kyongwan Kim, Tohoku University, AIMR |
| 17:00 ~ 17:40 | Dynamics of colloidal nanorods in a drying film | Narina Jung, UNIST |
| 18:00 ~ 20:00 | Dinner | |
| **Day 2: December 20, 2017** | | |
| **Time** | **Title** | **Speaker** |
| 09:00 ~ 10:00 | Special Lecture: Onsager's Principle 2 | Masao Doi, Beihang University |
| 10:00 ~ 10:40 | Switching mechanism in bent-core liquid crystal phases | Sookyung Joo, Old Dominion University |
| 10:40 ~ 10:50 | Coffee Break | |
| 10:50~ 11:30 | Cholesteric Lyotropic Chromonic Liquid Crystals: Effects of saddle-splay elastic modulus and dopants | Joonwoo Jeong, UNIST |
| 11:30~ 12:10 | Liquid crystalline Skyrmions and their direct optical observation | Jun-ichi Fukuda, |
| 12:00 ~ 13:30 | Lunch | |

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|---|---|---|
| 13:30 ~ 14:30 | CNU Interdisciplinary Distinguished Lecture Series: Mathematics of Patterns | Yasumasa Nishiura, Tohoku University, AIMR |
| 14:30 ~ 15:00 | Coffee Break | |
| 15:00 ~ 15:40 | Dynamics of liquid crystal phase transition in sedimenting platelet particles | Jize Sui, Beihang University |
| 15:40 ~ 16:20 | Architectures of Protein Nanotubes Triggered by Cationic Molec | Myung Chul Choi, KAIST |
| 16:20 ~ 17:00 | Phase Transition Line Runs to Widom Delta | Yongseok Jho, UNIST |
| 17:00 ~ 17:40 | A generalized finite volume method for density driven flow in porous media | Yueyuan Gao, Tohoku University, MathAM-OIL, AIST |
| 18:00 ~ 20:30 | Banquet | |
| **Day 3: December 21, 2017** | | |
| **Time** | **Title** | **Speaker** |
| 09:00 ~ 09:50 | Special Lecture: Onsager's Principle 3 | Masao Doi, Beihang University |
| 09:50 ~ 10:30 | Numerical simulations on adsorption of the surfactant | Yana Di, Chinese Academy of Science |
| 10:30 ~ 10:50 | Coffee Break | |
| 10:50 ~ 11:30 | Simulation Studies on Self-Assembly of Polymeric Systems: Thermodynamics vs. Kinetics | Su-Mi Hur, Chonnam National University |
| 11:30 ~ 12:10 | A structure-preserving finite element scheme for the Maxwell model | Hirofumi Notsu, Kanazawa University |
| 12:10 ~ 14:00 | Lunch | |
| 14:00 ~ 16:30 | Group Discussions | Natsuhiko Yoshinga, Tohoku University, AIMR |
| 16:30 ~ 17:30 | Discussion on Future Collaborations | Masao Doi, Jinhae Park, Natsuhiko Yoshinaga |

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| 17:30 ~17:40 | Closing remarks | Jinhae Park, Chungnam National University |
| 18:00 ~ 20:00 | Dinner | |

# Abstract

1. Masao Doi, Beihang University, China

2. The drying of liquid droplets (Xingkun Man, Beihang University, China)

Abstract: The drying of liquid droplets is a common daily life phenomenon that has long held a special interest in scientific research. We propose an Onsager variational principle theory that describes the droplet shape evolution and predicts the deposit distribution of nonvolatile components on the substrate. It is shown that for the drying of a single droplet, the deposition pattern changes continuously from a coffee ring to volcanolike and to mountainlike depending on the mobility of the contact line and the evaporation rate. When drying of two neighboring droplets, asymmetrical ring-like deposition patterns are formed, including fanlike and eclipse-like deposition patterns. The same theoretical model also explained the observed attraction-repulsion-chasing behaviors of evaporating droplets, where the droplets are not pinned. Evaporating droplets are known to show complex motion that has conventionally been explained by the Marangoni effect (flow induced by the gradient of surface tension). We show that the droplet motion can be induced even in the absence of the Marangoni effect due to the gradient of evaporation rate.

3. Novel dynamics in systems of microtubules and kinesin motor proteins (Kyongwan Kim, Tohoku University, AIMR)

   Microtubules (MTs) are dynamic cytoskeletal polymers and kinesin is a MT-associated motor protein. Polar nature of MTs, unidirectional processive motion of kinesin, and their nucleotide-controlled structurization and motility give rise to the ever-changing molecular machinery essential to cell life. We reconstitute these functionally paired proteins in a glass-cell chamber for fluorescence microscopy studies, emulating various situations similar to what they encounter in a cell. Charged nature of proteins, crowdedness, and geometrical boundary conditions are considered as cellular factors. Synthetic elements, such as quantum-dots and non-metallic/metallic glass microwires, are employed, to act as artificial cargos, cross-linkers, linear templates, or electrical signaling elements. In a regime of well separated proteins bound to a flat surface, the in-vitro MT-kinesin system retains sheer random-like kinesin-driven MT gliding or typical kinesin-assisted cargo transport along MT tracks. Likewise, large inter-protein spacing in a diluted solution suppresses any elaborate protein interaction, resulting in random fluctuation. Upon alteration of such circumstances to cell-like regimes in several aspects, however, the system reveals protein behavior quite distinctive. It is strongly coordinated with the structural and functional properties of the synthetic elements involved. Furthermore, increasing system crowdedness, in bulk as well as in a membranous arrangement, leads to long-range active coupling whose characteristic length scale is far beyond that of individual proteins. We will discuss various intriguing dynamics driven by the strongly coupled cytoskeletal proteins and synthetic organelles, putting forward potential applicability of the cellular mimetic approach to fundamental study, protein-based micro/nano-devices, and medical science.

4. Dynamics of colloidal nanorods in a drying film(Narina Jung, UNIST)

   We model the dynamics of self-assembly in drying nanorod solutions. The models include the kinetic interply among evaporation, shape dependent interaction between nanorods, and the excluded volume of nanorods. We investigate under which conditions nanorods self-assemble into the experimentally observed vertical alignment using a coarse grained method. We discuss first the isotropic-neumatic phase transition without evaporation and then the effects of evaporation rates, concentration and aspect ratios of nanorods on the self-assembly.

5. Switching mechanism in bent-core liquid crystal phases( Sookyung Joo, Old Dominion University, USA)

We describe the switching process in B1RevTilted and ferroelectric bistability of polarization-modulated orthogonal smectic liquid crystals (SmAP). The B1RevTilted is a uniformly smectic tilted columnar phase in which the macroscopic polarization can be reorientated via electric field. To study the effects on the reorientation mechanism of the various physical parameters, we analyze a Landau-de Gennes-type energy functional. For the case of large columnar samples, we show how the switching occurs with a relevant role played by the terms that describe the interaction between polarization and nematic directors. In SmAP phase, the opposite anchoring at the stripe boundaries and in-polarization form topological singularities. The free energy of the polarization with electric self-interaction term on one stripe reduces to the Ginzburg-Landau functional with boundary penalty term. We describe the boundary vortices of the reduced functional and obtain convergence results of minimizers. We also perform numerical simulations to illustrate the results of our analysis

6. Cholesteric Lyotropic Chromonic Liquid Crystals: Effects of saddle-splay elastic modulus and dopants (Joonwoo Jeong, UNIST)

   Water-based lyotropic chromonic liquid crystals (LCLCs) are materials of active study because of their biocompatibility and unusual elastic properties such as a very small twist elastic modulus and an unprecedentedly large saddle-splay elastic modulus. The unique elastic properties often result in spontaneous chiral symmetry breaking of confined achiral LCLCs, which leads to new types of chiral director configurations and topological defects. Here I share a series of experimental results elucidating how water-soluble chiral dopants added to LCLCs affect director configurations of confined LCLCs. First, we investigate director configurations of the cholesteric LCLCs confined within cylindrical capillaries and demonstrate the competing roles of the saddle-splay elastic modulus and helical twisting power of the chiral dopants added. Especially, when the helical pitch is comparable to the size of the capillary, the cholesteric LCLCs manifest strong effects of the saddle-splay elasticity and exhibit interesting topological defects. In addition to the cylindrical confinement, I introduce another chiral configuration arsing in the nematic-isotropic coexistence phase of the LCLCs.

7. Liquid crystalline Skyrmions and their direct optical observation(Jun-ichi Fukuda, Kyushu University, Japan)

   We show both theoretically and experimentally that Skyrmions, vortex-like excitations without singularities at the center, can form spontaneously in a thin film of a chiral liquid crystal. Skyrmions appear in the form of a hexagonal lattice or as isolated entities depending on the experimental conditions. We present our numerical results on the orientational order parameter profiles of Skyrmions, and their experimental and numerical microscope images.

8. Dynamics of liquid crystal phase transition in sedimenting platelet particles (Jize Sui, Beihang University, China)

   We report the dynamics of isotropic-nematic phase transitions in a dilute suspension consisting of rigid platelet-like particles by sedimentation. We employ Onsager variational principle (OVP) to determine the time evolution of the concentration and order parameter in space simultaneously on the basis of a simple free energy model effective for the anisometric particles with a range of aspect ratio

9. Architectures of Protein Nanotubes Triggered by Cationic Molecules (Myung Chul Choi, KAIST)

   Cells are working by well-designed molecular machines for a variety of tasks: to transfer the genetic blueprint, to move muscles, to transport nutrients, etc. Among them, microtubules (MTs) are involved in dividing cell, intracellular trafficking and defining call shape. MTs are 25 nm anionic protein nanotubes, comprised of globular dimeric tubulin subunits aligned end-to-end to form linear protofilaments, which interact laterally to form hollow cylinder. The structures and dynamics of MTs are rgulated by molecular switches, such as GTP, chemotherapeutic drug, microtubule-associated-proteins (MAPs), etc. This talk will deal with our recent findings on the assembly architectures of MTs triggered by cationic molecules using small angle X-ray scattering and electron micrography

10. Phase Transition Line Runs to Widom Delta (Yongseok Jho, UNIST)

MinYoung Ha, Tae Jun Yoon, Tsvi Tlusty*, YongSeok Jho*, WonBo Lee*

Although the macroscopic phase over critical point falls into a single supercritical fluid phase (SCF), interesting inhomogeneity in response functions have been observed. In this work, we show that this macroscopic change is originated from the microscopic configuration changes by using machine learning technique, which eventually classifies SCF into two local states: gas-like and liquid-like states. In this view point, the SCF is actually a mixture of inhomogeneous local states. And the abrupt divergence along the phase transition line broadened into finite and triangular area in SCF, like a river flowing into delta at sea (we call it "Widom delta".). According to this argument, we show that the Widom line can be interpreted as a part of Widom delta satisfying a particular condition.

11. A generalized finite volume method for density driven flow in porous media( Yueyuan Gao, Tohoku University, MathAM-OIL, AIST, Japan)

In this talk, we present numerical simulations for density driven flows in porous media. It amounts to solving a nonlinear convection-diffusion parabolic equation for the concentration coupled with an elliptic equation for the pressure. The pressure is derived from Darcy's law. We apply a semi-implicit time scheme together with a generalized finite volume method SUSHI [1], for which the orthogonality condition and volume matching condition of the mesh are not necessary. After presenting the generalized finite volume method SUSHI in the case of a linear elliptic problem, we perform numerical tests for porous media problems: the rotating interface problem and Henry's problem in space dimension two. These tests extend a paper by Hilhorst-Vu Do-Wang [2] where they apply the standard finite volume method.

This is joint work with Danielle Hilhorst and Huy Cuong Vu Do.

References:

[1] R. Eymard, T. Gallouët, R. Herbin. Discretization of heterogeneous and anisotropic diffusion problems on general nonconforming meshes SUSHI: a scheme using stabilization and hybrid interfaces. IMA J. Numer. Anal. 2010, 30(4), 1009-1043.

[2] D. Hilhorst, H. C. Vu Do and Y. Wang. A nite volume method for density driven flows in porous media. ESAIM: Proc. 2012, 38, 376-386.

12. Numerical simulations on adsorption of the surfactant (Yana Di, Chinese Academy of Science, China)

The research of surfactant systems is one of the important areas in soft condensed matter physics. The surfactant behaviors result in various kinds of interface/surface phenomena and also effect greatly on the physical characters of complex fluid systems. Here, we treat these problems in a physical way, and simulate the interface wetting and spreading phenomena of polydimethylsiloxane oil/ surfactant solution systems. We try to understand how the electrostatic/volume effect related to surface change the wetting status.

13. Simulation Studies on Self-Assembly of Polymeric Systems: Thermodynamics vs. Kinetics (Su-Mi Hur, Chonnam National University)

The self-assembly in polymeric system is one of core principles to many of advanced nanotechnologies. Success of most of these applications utilizing the self-assembly relies on how well one can adjust and switch the shape, size and arrangement direction of self-assembly. Hence there have been active research efforts in understanding the underlying physics and controlling the self-assembls4y, augmented by theoretical and numerical modeling. Complicated interactions, high sensitivity on various system parameters, wide range of length and time scales related with self-assembled structures make finding theoretical modeling very challenging. Moreover, in many systems, kinetics, and not only thermodynamics, plays a key role for the ability of a polymeric material to self-assemble into a desired state. However, a theoretical and numerical analysis of morphology formation in those systems is mostly unavailable due to the intrinsic non-equilibrium nature of those systems.

In this work, we present our efforts on developing efficient simulation approaches to describe the evolution of microstructure and the transformation between various microphases in block copolymer thin films. Our new numerical model, which can mimic an experimental solvent annealing, predict the self-assembled structure of block copolymer thin films in response to film swelling and solvent evaporation. We also use a combination of sampling technique named string method and a diffusive particle–based simulation to predict the kinetic path of defects in block copolymer thin film. Calculated minimum free energy pathway and the

corresponding free-energy barriers for eliminating defects provide the better understanding on the motion of defects and an explanation of experimental observations.

References

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W. Li, M. Muller, P. F. Nealey, J.J. de Pablo, PNAS, 112, 14144 (2015).

2. S. Hur, G.S. Khaira, A.R. Hernandez, M. Muller, P. F. Nealey, J.J. de Pablo, Macro Lett., 4, 11 (2015).

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14. A structure-preserving finite element scheme for the Maxwell model (Hirofumi Notsu, Kanazawa University)

In the talk, we study a numerical method for the Maxwell viscoelastic model in terms of the energy. Firstly, the gradient flow structure and the energy decay property of the model are presented. Secondly, for a time-discretized model, a corresponding discrete gradient flow structure is established and a time-discrete version of the energy decay property is derived from the structure. Thirdly, a structure-preserving finite element scheme is presented, where the stability in the sense of energy is ensured by the gradient flow structure and error estimates with the optimal convergence order are proved. Lastly, some numerical experiments are shown.