
2024 KIAS-FUB International Workshop
on Bio-Soft Matter Theory
Seoul, 20 - 23 Feb. 2024

PROGRAM

2024 KIAS-FUB International Workshop on Bio-Soft Matter Theory

Seoul, 20 - 23 Feb. 2024



Date and Place

20 Feb. 2024 (Tue.) - 23 Feb. 2024 (Fri.)
Seminar Room 1503, Building 1, Korea Institute for Advanced Study (KIAS)
85 Hoegiro, Dongdaemun-gu, Seoul 02455, Republic of Korea

Speakers

Ryo Akiyama
Kyushu University, Japan

Joachim Dzubiella
University of Freiburg, Germany

Tetsuya Hiraiwa
Academia Sinica, Taiwan

Changbong Hyeon
Korea Institute for Advanced Study (KIAS), Korea

Petra Imhof
Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Jae-Hyung Jeon
Pohang University of Science and Technology (POSTECH), Korea

Yong Seok Jho
Gyeong Sang National University, Korea

Narina Jung
Korea Institute for Advanced Study (KIAS), Korea

Matej Kanduč
Jozef Stefan Institute, Slovenia

Julian Kappler
Ludwig Maximilian University of Munich, Germany

Yong Woon Kim
Korea Advanced Institute of Science and Technology (KAIST), Korea

Susanne Liese
Universität Augsburg, Germany

Lei Liu
Zhejiang Sci-Tech University, China

Shavkat Mamatkulov
Institute of Materials Science of the Uzbekistan AS, Uzbekistan

Markus Miettinen
University of Bergen, Norway

Sebastian Milster
University of Freiburg, Germany

Arturo Moncho-Jordá
University of Granada, Spain

Roland R. Netz
Free University Berlin (FUB), Germany

Henri Orland
Université Paris-Saclay, France

Rudolf Podgornik
University of Chinese Academy of Sciences, China

Alexander Schlaich
University of Stuttgart, Germany

Taegeun Song
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Korea Institute for Advanced Study (KIAS)
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Korea Institute for Advanced Study (KIAS)
85 Hoegiro, Dongdaemun-gu, Seoul 02455, Republic of Korea

20 Feb. 2024 - 23 Feb. 2024

Program

	Feb. 20 (Tuesday)	Feb. 21 (Wednesday)	Feb. 22 (Thursday)	Feb. 23 (Friday)
09:00-09:30	Welcome & Registration	Coffee and breads		
09:30-10:20		Chair: M.Miettinen Matej Kanduč	Chair: S.Liese Rudolf Podgornik	Chair: M.Kanduč Petra Imhof
10:20-11:10		Susanne Liese	Henri Orland	Markus Miettinen
11:10-11:20		Break		
11:20-12:10		Yuki Uematsu	Alexander Schlaich	Jejoong Yoo
12:10-	Lunch			Closing Remarks
13:30-13:40	Opening Remarks			
13:40-14:30	Chair: W.K.Kim Narina Jung	Chair: A.Schlaich Roland R. Netz	Ryo Akiyama	Excursion (Seoul Palaces & N Seoul Tower & Dinner)
14:30-15:20	Lei Liu	Julian Kappler	Chair: T. Hiraiwa Joachim Dzubiella	
15:20-15:30	Break			
15:30-16:20	Changbong Hyeon	Yong Woon Kim	Arturo Moncho-Jorda	
16:20-17:10	Chair: W.K.Kim YongSeok Jho	Jae-Hyung Jeon	Xiao Xu	
17:10-17:20	Break			
17:20-18:10	Taegeun Song	Tetsuya Hiraiwa	Sebastian Milster	
18:10-	Dinner	Poster session / Pizza	Banquet	

Feb. 20 (Tuesday)

Polymers and flagella

Chair: Won Kyu Kim

13:40-14:30

Narina Jung Korea Institute for Advanced Study (KIAS), Korea

The collective behaviors of active filaments

To investigate the collective behaviors of an array of active filaments coupled through hydrodynamic and steric interactions, we consider identical elastic filaments that undulate transversely in a confined viscous fluid. We study the impact of tilting angles on the formation of metachronal waves that break the transversal symmetry in the governing equations. We first show that for two filaments placed side by side, increasing the longitudinal displacement of their head positions leads to a breakdown of whole body synchronization, transitioning to synchronization of their overlapped bodies, and then gradually to decoupled dynamics. When examining an array of tilted filaments, whole-body synchronization can emerge despite longitudinal displacement, but it exhibits a constant time delay that increases with the tilt angle. Consequently, it leads to a traveling metachronal wave propagating from filament to filament.

14:30-15:20

Lei Liu Zhejiang Sci-Tech University, China

Constructing full genome architecture with a Hi-C guided many-polymer model

High-throughput chromosome conformation capture (Hi-C) is arguably the most efficient and cost-effective method in genome research to collect information on three-dimensional (3D) genome structure. Over the past years, a growing amount of Hi-C data for various cell types and species have been deposited and made accessible to the public. Here we suggest a many-polymer model to reconstruct 3D full genome structures using Hi-C as the sole input without additional constraints from other imaging or biochemical assays. Applications of this method to seven different species encompassing animalia, plantae, and fungi demonstrate its great versatility in reconstructing and studying the high-order 3D organization of complete genome.

15:30-16:20

Changbong Hyeon Korea Institute for Advanced Study (KIAS), Korea

Irregularity of polymer domain boundaries in 2D polymer solution

Data-driven studies on bio-soft matter

Chair: Won Kyu Kim

16:20-17:10

YongSeok Jho Gyeong Sang National University, Korea

Li ion transport in ionic liquid

17:20-18:10

Taegeun Song Kongju National University, Korea

Breaking new ground: collaboration of physics and A.I.

Feb. 21 (Wednesday)

Water and bubbles

Chair: Markus Miettinen

09:30-10:20

Matej Kanduč Jozef Stefan Institute, Slovenia

Tiny hydrophobic matter with huge consequences

Hydrophobic interaction, a fundamental force in biophysics, has a long and venerable history of research, yet it remains enigmatic. Its impact can sometimes be profound: Even minute traces of hydrophobic matter within an otherwise pure aqueous system can shape its behavior. In this presentation, I will explore two intriguing scenarios that shed light on this phenomenon. Firstly, I will discuss why hydrophilic surfaces in water can attract all the way down to a contact angle of 65°, known as the Berg limit. This universal contact angle poses a challenge to conventional theories, which struggle to explain hydrophobic interactions between hydrophilic surfaces. The other puzzling question I will investigate is why water is so unstable against cavitation and vaporization. While theoretical predictions suggest water should be highly stable, experiments show quite the opposite. Through computer simulations, we have demonstrated that even a single nanoscopic hydrophobic defect on a surface or a tiny nanodroplet of organic contaminants suspended in water can initiate nucleation and destabilize an entire, otherwise resilient, macroscopic aqueous system. These outcomes illuminate how hydrophobic interactions affect water behavior, carrying broad scientific implications.

10:20-11:10

Susanne Liese Universität Augsburg, Germany

Chemically active wetting

Wetting of liquid drops is not only ubiquitous in our daily life, the underlying physics also plays a crucial role in living cells. Droplets composed of proteins can wet specific target sites on cellular surfaces and locally enrich biomolecules for specific chemical processes. Many droplet-forming proteins can also bind to membrane surfaces. Binding in cells is often chemically active maintained away from equilibrium which can in turn alter the laws of wetting. Here we derive the non-equilibrium thermodynamic theory for active wetting. By means of this theory, we show that active binding fundamentally changes the wetting behavior leading to non-equilibrium steady states with condensate shapes reminiscent of a fried egg or a mushroom. The origin of such anomalous condensate shapes can be explained by an electrostatic analogy, where binding sinks and sources correspond to electrostatic dipoles along the triple line. This analogy suggests a general analogy between chemically active systems and electrodynamics.

11:20-12:10

Yuki Uematsu Kyushu Institute of Technology, Japan

Ostwald ripening of aqueous microbubble solutions

The kinetics of radii in aqueous microbubble solutions are experimentally investigated, and the results are discussed in the context of Ostwald ripening. The obtained distributions of bubble radii scaled by mean radius and total number were found to be time-independent during the observation period. Image analysis of radii kinetics revealed that the average growth and shrinkage speed of each bubble is governed by diffusion-limited Ostwald ripening, and the kinetic coefficient calculated using the available physicochemical constants in the literature quantitatively agrees with the experimental data.

Stochasticity and non-equilibrium dynamics in bio-soft matter

Chair: Alexander Schlaich

13:40-14:30

Roland R. Netz Free University Berlin, Germany

Systematic approaches to non-equilibrium systems

The dynamics of many-body systems, when described in terms of a low-dimensional reaction coordinate, is governed by the generalized Langevin equation (GLE). The GLE is an integro-differential stochastic equation and involves a memory function, which describes how the reaction coordinate dynamics depends on its previous values. The GLE is an accurate coarse-grained non-Markovian description of the system dynamics, as has been demonstrated for molecular conformations [1], vibrational spectroscopy [2], chemical reactions [3] and protein folding [4]. The proper coarse-grained description of the dynamics of non-equilibrium driven systems, characterized by a time-dependent Hamiltonian and by slowly relaxing transient variables, is less developed. Two systematic approaches for such systems are discussed: Using an appropriate projection for a time-dependent Hamiltonian system, an exact non-equilibrium GLE is derived [5]. This GLE illustrates the intricate coupling of non-linear and non-Markovian effects. As an alternative approach, data filtering is shown to lead to modified GLEs that are particularly useful for the treatment of time series data from non-physical sciences. As a practical application, results for weather prediction are presented.

[1] Generalized Langevin equation with a nonlinear potential of mean force and nonlinear memory friction from a hybrid projection scheme, Cihan Ayaz , Laura Scalfi , Benjamin A. Dalton, Roland R. Netz, PHYSICAL REVIEW E 105, 054138 (2022), DOI: 10.1103/PhysRevE.105.054138
[2] Time-Dependent Friction Effects on Vibrational Infrared Frequencies and Line Shapes of Liquid Water, Florian N. Brünig, Otto Geburtig, Alexander von Canal, Julian Kappler, Roland R. Netz, J. Phys. Chem. B 2022, 126, 1579−1589, DOI: 10.1021/acs.jpcb.1c09481
[3] Pair-Reaction Dynamics in Water: Competition of Memory, Potential Shape, and Inertial Effects, Florian N. Brünig, Jan O. Daldrop, Roland R. Netz, J. Phys. Chem. B 2022, 126, 10295−10304, DOI: 10.1021/acs.jpcb.2c05923
[4] Fast protein folding is governed by memory-dependent friction, Benjamin A. Dalton, Cihan Ayaz, Lucas Tepper, and Roland R. Netz,
Proc. Natl Acad. Sci. 120, e2220068120 (2023), DOI: 10.1073/pnas.2220068120
[5] Derivation of the non-equilibrium generalized Langevin equation from a generic time-dependent Hamiltonian, Roland R. Netz,
https://arxiv.org/abs/2310.00748

14:30-15:20

Julian Kappler Ludwig Maximilian University of Munich, Germany

Stochastic action for tubes: connecting path probabilities to measurement

Stochastic effects are ubiquitous in physical systems, and are widely modeled by diffusion processes. The trajectories of diffusion processes are continuous but nondifferentiable, and each occurs with vanishing probability. This introduces a gap between theory, where path probabilities are used in many contexts, and experiment, where only events with nonzero probability are measurable. We bridge this gap by considering the probability of diffusive trajectories to remain within a tube of small but finite radius around a smooth path. This probability can be measured in experiment, via the rate at which trajectories exit the tube for the first time, thereby establishing a link between path probabilities and physical observables. In my talk I will show how this link can be used to both measure ratios of path probabilities, and to extend the theoretical stochastic action from individual paths to tubes. I will furthermore discuss the scenario where the diffusivity is state-dependent.

15:30-16:20

Yong Woon Kim Korea Advanced Institute of Science and Technology (KAIST), Korea

Active search for a reactive target

We study a stochastic process where an active particle, modeled by a one-dimensional run-and-tumble particle, searches for a target with a finite absorption strength in thermal environments. Solving the Fokker-Planck equation for a uniform initial distribution, we analytically calculate the mean searching time (MST), the time for the active particle to be finally absorbed, and show that there exists an optimal self-propulsion velocity of the active particle at which MST is minimized. As the diffusion constant increases, the optimal velocity changes from a finite value to zero, which implies that a purely diffusive Brownian motion outperforms an active motion in terms of searching time. Depending on the absorption strength of the target, the transition of the optimal velocity becomes either continuous or discontinuous, which can be

understood based on the Landau approach. In addition, we obtain the phase diagram indicating the passive-efficient and the active-efficient regions. Finally, the initial condition dependence of MST is presented in limiting cases.

16:20-17:10

Jae-Hyung Jeon Pohang University of Science and Technology (POSTECH) & Asia Pacific Center for Theoretical Physics (APCTP), Korea

Nonequilibrium viscoelastic diffusion modeled by active fractional Langevin equations

17:20-18:10

Tetsuya Hiraiwa Institute of Physics, Academia Sinica, Taiwan

Dynamic self-organization of migrating cells

Migratory behavior is a ubiquitous kind of eukaryotic cell dynamics. When migrating cells communicate with each other and act in union, they can exhibit varieties of dynamic patterns and coherent motion (dynamic self-organization). In this presentation, we discuss what forms of dynamic self-organization of migrating cells are caused through contact communication between cells theoretically [1]. After looking through single-cell migratory behavior and its theoretical model [2,3], the theoretical model for cell collectives based on an individual cell dynamics-based model in which migrating cells perform two ubiquitous types of contact communication, called contact following and contact inhibition of locomotion, and the numerical simulation results of this model are explained [1]. Some results are compared with experimental observations of dynamic patterns shown by some living cells [4]. In addition, how such dynamic self-organization can play roles for functional behaviors, like accurate directional migration and mobility under constraints, is explained [1,5,6].

[1] T. Hiraiwa, PRL 125, 268104 (2020).
[2] T. Hiraiwa, A. Nagamatsu et al., Phys. Biol. 11, 056002 (2014).
[3] T. Hiraiwa, A. Baba et al. EPJE 36, 32 (2013).
[4] M. Hayakawa, T. Hiraiwa et al., eLife 9, e53609 (2020).
[5] T. Hiraiwa, PRE 99, 012614 (2019).
[6] T. Hiraiwa, EPJE 45, 1 (2022).

Poster session

Ryo Akiyama Department of Chemistry, Kyushu University, Japan
A theoretical approach for separation device based on the idea of entropic attraction

Hyeong-Tark Han POSTECH, Korea
Nonequilibrium diffusion of active particles bound to a semi-flexible polymer network: simulation and fractional Langevin equation

Tomoya Iwashita Department of Chemistry, Kyushu University, Japan
Molecular dynamics study of difference of friction coefficients between hydrophilic and hydrophobic surfaces on a macromolecule in water

Minsoo Kim Sungkyunkwan University, Korea
Multi-gpu implementation of Alphafold

Yeongjin Kim POSTECH, Korea
Active diffusion of self-propelled particles in flexible and semi-flexible polymer networks

YeongKyu Lee Gyeongsang National University, Korea
Divergence of differential capacitance at electrode: statistical field theory with Coulomb and Yukawa potentials

O-chul Lee Department of physics, POSTECH, Korea
State classification of xpc`s one-dimensional heterogeneous diffusion using GMM and HMM

Chan Lim POSTECH, Korea
Transient anomalous diffusion in a viscoelastic media: a coupled fractional Langevin equation approach

Markus Miettinen Computational Biology Unit, Department of Chemistry, University of Bergen, Norway
Virtual-deformation approach to obtain elastic properties of particle-based systems

Pyeong Jun Park KNUT, Korea
Fast calculation of long range interaction by artificial neural network

Daeseong Yong Center for AI and Natural Sciences, KIAS, Korea
Accelerating langevin field-theoretic simulation of block copolymers with deep learning

Ji Woong Yu Center for AI and Natural Sciences, KIAS, Korea
An investigation of anomalous water dynamics using a machine learning force field

Feb. 22 (Thursday)

Charged soft matter

Chair: Susanne Liese

09:30-10:20

Rudolf Podgornik University of Chinese Academy of Sciences, China

Electrostatic interactions between charge regulated spherical macroions

I will present new results on the interaction between two charge regulating spherical macroions with dielectric interior and dissociable surface groups immersed in a monovalent electrolyte solution, where the charge dissociation model allows for multiple adsorption equilibrium states. The interactions are derived from the solutions of the mean-field Poisson-Boltzmann type theory with charge regulation boundary conditions. For a range of conditions we find symmetry breaking transitions from symmetric to asymmetric charge distribution exhibiting annealed charge patchiness, which results in like-charge attraction even in a univalent electrolyte—thus fundamentally modifying the nature of electrostatic interactions in charge-stabilized colloidal suspensions.

10:20-11:10

Henri Orland Institut de Physique Théorique, CEA, Université Paris-Saclay, France

Conductivity of concentrated ionic solutions

11:20-12:10

Alexander Schlaich SC SimTech, University of Stuttgart, Germany

Bio-inspired electrodes: from nano-pores to semi-conducting polymers

Nature has developed efficiency for biocatalysts that employ confining geometries of defined size, polarity (gradients) and tortuosity that accomplish reactions unreached by scientific discovery. In this talk I will discuss how nano-porous electrodes can not only serve for the emerging field of energy storage, but also increase efficiency for heterogeneous catalysis through confinement effects. Furthermore, the composition and dynamics of the confined species is strongly affected, which I will highlight for the environmentally relevant case of soil precipitation. I will conclude with an outlook on the ion dynamics in confining biocompatible semi-conducting polymers.

13:40-14:30

Ryo Akiyama Department of Chemistry, Kyushu University, Japan

Reentrant behavior in effective interactions between like-charged macroions immersed in an electrolyte solution

Effective interaction between like-charged macroions immersed in an electrolyte solution depends on the electrolyte concentration. Several experiments have shown the reentrant effective interaction change. For example, reentrant condensation behaviors of acidic proteins, which are negatively charged macromolecules, are shown in an electrolyte solution that contains multivalent cations. The experimental results show that the effective interaction becomes attractive only in a certain electrolyte concentration. We will show the reentrant behavior on the effective interaction using the integral equation theory and the molecular simulation and discuss the reentrant behavior.

Gels and colloids

Chair: Tetsuya Hiraiwa

14:30-15:20

Joachim Dzubiella Department of Physics, University of Freiburg, Germany

Modeling chemically fueled soft matter

Chemical fueling of soft matter, such as polymer, colloids, or liquids, leads to interesting nonequilibrium states and the possibility to design programmable and adaptive soft functional materials. Here, I discuss a few models and simulations of the chemical fueling of simple soft matter systems, such as dispersions of colloidal hydrogels or simple liquids displaying transient behavior - such as intermediate collapsed or cluster states - in the time domain. I highlight the role of feedback mechanisms which lead to much richer dynamics, enabling the synthesis of well-controlled excitable media.

15:30-16:20

Arturo Moncho-Jorda Department of Applied Physics. University of Granada, Spain

Non-equilibrium active interaction switching of soft colloids: microstructure, phase behaviour and heterogeneous dynamics

We explore the microstructure and phase behavior of a nonequilibrium system comprised by soft colloids that can actively switch their interactions between two states at a predefined kinetic rate. For this purpose, we employ a Reactive Dynamical Density Functional Theory (R-DDFT) and reactive Brownian-Dynamics simulations (R-BD). We find that the switching rate interpolates between a near-equilibrium binary mixture at low rates and a nonequilibrium monodisperse liquid for large rates, strongly affecting the one-body density profiles, adsorption, and pressure at confining walls. Importantly, we show that sufficiently fast switching impedes the phase separation of an (in equilibrium) unstable liquid, allowing the control of the degree of mixing and condensation and local microstructuring in a cellular confinement by tuning the switching rate [1, 2]. Switching activity also modifies the dynamics and diffusion coefficients of the individual particles, leading to a crossover from short to long times, with a regime for intermediate times showing anomalous diffusion [3]. The corresponding self-intermediate scattering function shows the two-step relaxation patters typically observed in soft materials with heterogeneous dynamics such as glasses and gels. R-DDFT results are in excellent agreement with R-BD simulations and the analytical predictions of a phenomenological Continuous Time Random theory, thus confirming that R-DDFT constitutes a powerful method to investigate not only the structure and phase behavior, but also the dynamical properties of non-equilibrium active switching colloidal suspensions.

Acknowledgements: We thank the ""Plan Estatal de Investigación Científica, Técnica y de Innovación"" (Project PID2022-136540NB-I00).

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[2] M. Bley, J. Dzubiella and A. Moncho-Jordá, Soft Matter, 2021, 17, 7682.
[3] M. Bley, P.I. Hurtado, J. Dzubiella and A. Moncho-Jordá, Soft Matter, 2022, 18, 397

16:20-17:10

Xiao Xu Nanjing University of Science and Technology, China

Binding of proteins to copolymers of varying charge and hydrophobicity: a molecular mechanism and computational strategies

Because of their ability to selectively bind to a target protein, copolymer nanoparticles (NPs) containing a selected combination of hydrophobic and charged groups have been frequently reported as potent antibody-like analogues. However, due to the intrinsic disorder of the copolymer NP in terms of its random monomer sequence and the cross-linked copolymer matrix, the copolymer NP is indeed strikingly different from a well-folded antibody protein and the complexation between the copolymer NP and a target protein is likely not due to a lock-key type of interaction but possibly due to a novel and unexplored molecular mechanism. Here, we study a key biomarker protein, vimentin, interacting with a set of random copolymer chains using implicit-water explicit-ions coarse-grained (CG) molecular dynamics (MD) simulations along with biolayer interferometry (BLI) analysis. Due to the charge and hydrophobicity anisotropy on the vimentin dimer (VD) surface, a set of bound copolymers are found inhomogeneously adsorbed on the VD, with energetic heterogeneity for different binding sites and cooperative effect in the adsorption. Increasing the charge or hydrophobicity of the copolymer may have different consequences on the adsorption. In this study, we found that with more copolymer charges, the protein coverage increases for copolymers of low hydrophobicity and decreases of high hydrophobicity, which is explained by the distribution and size of various functional patches on the VD in loading those copolymers. Employing a coverage-dependent Langmuir

model, we propose a simulation protocol to address the full profile of the copolymer binding free energy through the fit to the simulated binding isotherm. The obtained results correlate well with those from BLI experiment, indicating the significance of this method for the rational design of the copolymer NP with engineered protein binding affinity.

17:20-18:10

Sebastian Milster Department of Physics, University of Freiburg, Germany

Tracer friction and memory in polymer networks

This work is concerned with the dynamics of small molecules in a fluctuating polymeric environment. We employ Langevin simulations of bead-spring polymer networks, containing spherical tracer solutes. We analyze autocorrelation functions and friction memory kernels for different tracer--network interaction strengths. We recover the long-time transport coefficients from various methods, and identify the network dynamics governing the tracer friction and memory on multiple timescales.

Feb. 23 (Friday)

Atom-level computational studies on bio-soft matter

Chair: Matej Kanduč

09:30-10:20

Petra Imhof Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Effect of inter- and intramolecular interactions on conformational dynamics and reactivity

The geometric and electronic structure of molecular systems can be significantly influenced by their environment. This can be the surrounding solvent, a (large) host molecule or catalyst, reaction partners or, other parts of the molecule itself. Many chemical processes take place in the liquid phase, and hence, the knowledge about the impact of solute-solvent interactions and balance with solute-solute interactions is crucial for the interpretation and prediction of molecular structure and properties. By employing molecular dynamics (MD) simulations for conformational sampling and molecular fragmentation, on extracted snapshots, we can calculate inter- and intramolecular interaction energies and determine structural changes of the solute molecule induced by the solvent. Furthermore, the effect on the vibrational signatures of the solute molecules can be quantified.

10:20-11:10

Markus Miettinen Computational Biology Unit, Department of Chemistry, University of Bergen, Norway

Integrative determination of the atomic structure of mutant huntingtin exon 1 fibrils from Huntington's disease

Neurodegeneration in Huntington's disease (HD) is accompanied by the aggregation of fragments of the mutant huntingtin protein, a biomarker of disease progression. A particular pathogenic role has been attributed to the aggregation-prone huntingtin exon 1 (HttEx1) fragment, whose polyglutamine (polyQ) segment is expanded. Unlike amyloid fibrils from Parkinson's and Alzheimer's diseases, the atomic-level structure of HttEx1 fibrils has remained unknown, limiting diagnostic and treatment efforts. We present and analyze the structure of fibrils formed by polyQ peptides and polyQ-expanded HttEx1. Atomic-resolution perspectives are enabled by an integrative analysis and unrestrained all-atom molecular dynamics (MD) simulations incorporating experimental data from electron microscopy (EM), solid-state NMR, and other techniques. Visualizing the HttEx1 subdomains in atomic detail helps explaining the biological properties of these protein aggregates, as well as paves the way for targeting them for detection and degradation.

11:20-12:10

Jejoong Yoo SungKyunKwan University, Korea

Developments of very accurate force field for the complexes of protein, DNA, and lipid molecules

As modern molecular dynamics simulation studies focus on increasingly complex systems of proteins, DNA/RNA, and lipid molecules in either structured or disordered states, it has been revealed that the molecular force fields such as AMBER and CHARMM are significantly limited in their accuracies. In this talk, I will introduce our strategy to improve the AMBER force field based on the thermodynamic properties of small solutes. Then, I will demonstrate that our improved force field (termed CUFIX-AMBER) dramatically improves the agreements with experiments for various biological systems including protein folding, intrinsically disordered proteins, protein-DNA complexes, and protein-lipid complexes.