2018년

CDLC Symposium

Statistical Thermodynamics for Small Chemical Systems

일시: 2018년 03월 21일(수) 14:00~18:30

장소: 중앙대학교 서울캠퍼스 310관 B 119호

주최: 세포화학동력학 창의연구단 (Center for Chemical Dynamics in Living Cells)

CDLC Creative Research Initiative
Center for Chemical Dynamics in Living Cells
National Research Foundation of Korea

프로그램

2018 년 3 월 21 일 수요일

Statistical Thermodynamics for Small Chemical Systems	
14:00 - 14:40	장준경 교수(부산대) Phase transitions of confined water: theory and simulation studies
14:40 - 15:20	황현석 교수(강원대) Exploring Interactions of Proteins and Surfactants with Biological Interfaces
15:20 - 16:00	장락우 교수(광운대) Inhibition Mechanism of TEX14 in Cell Division: Well-Tempered Metadynamics
16:00 - 16:10	Break Time
16:10 - 16:50	이영민 교수(KAIST) Excited State Energy Fluctuations in the Fenna-Matthews-Olson Complex: Distinction between Static and Dynamic Disorder through Molecular Dynamics Simulations
16:50 - 17:30	김준수 교수(이화여대) *in silico* exploration of new molecular systems
17:30 - 18:10	김지현 교수(중앙대) Handling Hidden yet Vital Factors: Novel Stochastic Kinetics for Complex Systems
18:10 - 18:30	성재영 교수 (중앙대) Closing remarks

구두발표 초록

Phase transitions of confined water: theory and simulation studies

Joonkyung Jang

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We present a theory for the wetting transition of the grooves engraved on a hydrophobic surface. We present a continuum theory for the free energy profile with respect to the level of liquid filling into the grooves. We investigate how the wetting transition depends on the shape and size of the grooves. Using Monte Carlo (MC) and molecular dynamics (MD) simulations, we investigate various intermediate states in the continuous wetting of the grooves, including the stable and metastable states, and transition states and activation energies. We developed an analytic theory to predict the stable state for simple geometries of grooves. This theory agreed with the molecular simulations, even for nanoscale grooves. We also report a large scale MD simulation study of the wettability of a gold surface engraved with spherical cavities.

Exploring Interactions of Proteins and Surfactants with Biological Interfaces

Hyonseok Hwang

Department of Chemistry, Kangwon National University

Interactions of bio- and nano- molecules with biological Interfaces play a key role in metabolism in cells. In this talk, I will present three different types of interactions between proteins or surfactants with biological interfaces. In the first part, energetic and dynamics of transport of Na+ and K+ through a cyclic peptide nanotube are addressed. Potential of mean force (PMF) profiles and position-dependent diffusion coefficients of Na+ and K+ are calculated to elucidate the translocation of ions through a cyclic peptide nanotube, composed of 8 × cyclo[-(D-Leu-Trp)4-] rings, in water and in hydrated DMPC bilayers. In the second part, we examine the thermodynamic and structural properties of Gram-negative outer membranes using all-atom molecular dynamics simulations. In the last, several issues on the micelle formation of a type of surfactants and insertion of micelles into ceramide bilayers are briefly addressed.

Inhibition Mechanism of TEX14 in Cell Division: Well-Tempered Metadynamics

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Cytokinesis is the process in which the cytoplasm is divided into two daughter cells after nuclear division in the cell division. In somatic cells, cytokinesis requires ALIX (or TSG101) and the midbody protein centrosomal protein (CEP55) to activate cell abscission. In germ cells, in contrast, CEP55 forms intercellular bridges with testis-expressed gene 14 (TEX14), by which the cell abscission is blocked. These intercellular bridges also play important roles in synchronization of germ cells, especially in spermatogenesis, by passage of organelles and molecules between germ cells. So, if TEX14 is deleted intentionally, intercellular bridges are disrupted, leading to sterility. These functions of TEX14 may provide information in the inactivation of the abscission to suppress the proliferation of cancer cells. Previous experimental studies showed that a high affinity and a low dissociation rate of TEX14 to CEP55 via the AxGPPx3YxPP (Ala793, Gly795, Pro796, Pro797, Tyr801, Pro803 and Pro804) motif of TEX14 prevents ALIX from binding and inactivates the germ cell abscission. However, the detailed information about how TEX14 interacts with CEP55 to prevent the cell abscission is still insufficient. Hence, to obtain more specific details about the interaction between CEP55 and TEX14, which is not easy to identify in experiments, we performed metadynamics simulations using atomistic models of CEP55 and TEX14.

Our results show that the Tyr801 residue of TEX14 binds to CEP55 stronger than other residues of TEX14 by forming a strong hydrogen bond with Glu192 residue of CEP55, which is consistent with previous experimental studies. The binding Gibbs free energy surface calculated by the metadynamics simulation is also in good agreements with experimental data. In the future, we plan to study other peptides containing the AxGPPx3YxPP motif of TEX14 as a candidate for the suppressor of cancer cell proliferation.

Excited State Energy Fluctuations in the Fenna-Matthews-Olson Complex: Distinction between Static and Dynamic Disorder through Molecular Dynamics Simulations

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By performing 100 ns long molecular dynamics simulations, we analyze the environment-induced fluctuations of pigment excitation energies in the Fenna-Matthews-Olson (FMO) complex from various respects. This is achieved by employing interpolation-based all-atom potential energy model for describing realistic pigment vibrations. The timescale can enclose the effect of static disorder as well as dynamic disorder. By a simple analysis, we demonstrate the timescale separation between the two aspects. We extract the spectral densities of the complex by considering both the site and the exciton bases. We show that exciton delocalization reduces the effective environmental fluctuation and rationalize this aspect based on a model of fluctuating molecular aggregate. We also obtained the spectral density of the lowest exciton state at a low temperature condition and show that it reasonably well reproduces the experimental result. Finally, by additionally performing non-equilibrium excited state trajectory simulations, we show that the system lies well within the linear response regime after photo-absorption and that the pigments do not visit anharmonic regions of the potential surface to a significant extent. This indicates that methodologies based on harmonic bath models are indeed reasonable approaches for describing the excited state dynamics, at least for the FMO complex studied here.

in silico exploration of new molecular systems

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In broad areas in science and engineering, computational physical chemistry has played important roles in interpreting experimental observations and finding basic principles underlying the physico-chemical processes. Another important, but less explored, role of computational physical chemistry is to explore and predict new chemical processes inaccessible by other experimental methods. We present our efforts to propose new molecular systems that may find great utility in future experimental approaches. Two examples include the conformational control of DNA molecules in an array of nanoposts and the directional transport of nanoparticles along a long DNA molecule. As well as mechanisms underlying these processes, their possible utilities will be discussed.

Handling Hidden yet Vital Factors: Novel Stochastic Kinetics for Complex Systems

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Gene expression is a complex stochastic process composed of numerous enzymatic reactions with rates coupled to hidden cell-state variables. Despite advances in single-cell technologies, the lack of a theory accurately describing the gene expression process has restricted a robust, quantitative understanding of gene expression variability among cells. Here we present a novel stochastic kinetics for living cells, providing an accurate relationship between the environment-coupled chemical dynamics of gene expression and gene expression variability. Combined with a general, accurate model of environment-coupled transcription and translation processes, we provide a unified, quantitative explanation of various gene expression statistics observed across a number of experimental systems. This work suggests promising new directions for quantitative investigation into not only cellular control over biological functions but also heterogeneous activity of single clonal enzymes and universal transport dynamics of complex fluids.